THE ROLE OF RISK IN CHEMICAL SUBSTITUTION DECISIONS

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THE ROLE OF RISK IN CHEMICAL SUBSTITUTION DECISIONS

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Executive Summary

Chemical substitution is a growing method of pollution prevention and toxics use reduction (TUR). Although a good deal of effort has gone into developing protocols for identifying potential substitutes, much less attention has been given to explicit identification and weighing of the health and environmental risks of alternative chemicals. This project focuses on the use of the tools of risk analysis in chemical substitution decisions. First, the way in which companies currently make substitution decisions is characterized from interviews with selected firms. Then proposed methods for chemical substitution are evaluated with particular attention to the role of risk in the schemes. Finally, a logic tree-based framework for evaluating the risks of alternative chemicals is proposed and discussed.

Many considerations play a role as companies confront chemical substitution decisions encouraged by pollution prevention activities or TUR requirements. From the interviews it is clear that the most important factors are regulatory compliance and cost. Firms strive to make substitutions that will avoid the many lists of chemicals which drive environmental laws such as Title III of the Superfund Amendments and Reauthorization Act (the toxics release inventory (TRI)) or the Massachusetts Toxics Use Reduction Act. In addition, they look for the lowest cost substitute. Factors such as performance, availability, and proven success in similar applications play a smaller role. Risk to the health of workers, the public, or the environment is rarely considered. Most firms seem to believe that through regulatory compliance and by avoiding listed toxic chemicals they are assured of risk reduction.

This perception that moving to unlisted chemicals will decrease risk also underlies the consideration of risk in most proposed chemical substitution schemes. Most focus on the identification of substitute chemicals or processes to reduce or eliminate the use of a target chemical. It is recognized that a substitute chemical may have health risks but it is generally assumed the chemicals not under regulatory scrutiny are safer than those that are.

The substitute evaluation protocol proposed here, the chemical substitution tree (CST), does not accept the premise that list based decisions will always reduce risk. It recognizes that all compounds can be toxic and that it is important to consider both exposure and the hazard potential of alternative chemicals to ensure risk reduction. It recognizes that few regulatory lists have a consistent risk or toxicological basis and that many have little concern for environmental or ecological hazards. Instead, it encourages companies to explicitly evaluate the potential risks to human and environmental health as an input to chemical substitution decisions.
Chemical substitution is a multiattribute problem with fundamentally incomparable metrics. It requires judgment to weigh cost, performance, risk, and other factors in making a substitution choice. For this reason no rigid, prescribed protocol for decision making can be constructed. What is needed, then, is not a highly regimented checklist type approach to substitution but rather the development of a decision making framework which explicitly considers the health, safety, and ecological risks of alternative chemicals in a substitution decision.

The goal of the chemical substitution tree is to encourage firms to explicitly consider the risk attributes of substitutes as an input to more informed decisions. The CST identifies both the exposure and hazard properties of a substitute compound and compares them to that of the chemical already in use (the base case chemical). Use of comparison simplifies the consideration of risks because relative risk will be easier to assess than absolute risk for any specific attribute. It encourages evaluation of exposure through the lifecycle of a chemical with a special emphasis on use and disposal. It focuses on chemical use on an application by application basis, recognizing that the risk, and opportunities for risk reduction, vary according to how a chemical is used. The CST asks firms to consider the hazards that the base case and substitute chemical may pose to worker health and safety, public health and safety, and the local and global environments.

The advantages of the CST approach are many. It makes clear the relative health, safety, and environmental attributes of substitute chemicals. It allows identification of problem areas, for example potential ecological risks of an otherwise less hazardous substance. The consideration of both exposure and hazard means that risk reduction opportunities can be identified. For example, preventing release to the environment may make a substitute be judged as superior because it removes the exposure responsible for significant risk. The main strength of the CST approach is that it is a flexible process that will lead to more informed decision making and will help achieve the goal of pollution prevention, risk reduction.

There are some current implementation problems with the CST approach. The most significant is the asymmetry of data quantity and quality for base case and substitute chemicals. Clearly, chemicals which are on regulatory lists of concern frequently have much more extensive toxicological information than those chemicals not on lists. The use of the CST, however, may be an incentive to increase the amount of information about substitutes and to improve methods of characterizing risk with limited information. Another possible drawback is that use of the CST method may increase the time and resource requirements for substitution decisions. It may
well be, on the other hand, that the effort to better inform the substitution decision will avoid the situation in which another substitution must be implemented because the first was made in haste.

Recommendations
1. Firms should be encouraged to use the CST framework when making chemical substitution decisions. When appropriate, companies should be encouraged to share documentation and results of the process.

2. An important need is the development of an information infrastructure to help companies in using the protocol. A central source of information, such as the Toxics Use Reduction Institute or Office of Technical Assistance in Massachusetts, or the Environmental Protection Agency nationally, is vital. For example, these groups could be sources for quantitative structure-activity relationship (QSAR) data for untested compounds as well as examples of potential substitutes.

3. Reliance on lists of toxic chemicals should be reduced. The goal of pollution prevention and toxics use reduction is risk reduction. Explicit evaluation of risk means that lists of chemicals of concern will not be necessary and may be counterproductive by removing from consideration chemicals which may allow significant risk reduction. Further experience with the CST approach, with explicit consideration of risk, will allow reduced reliance on lists of toxic chemicals and instead will open the entire universe of chemistry for substitution so that all risk reducing options may be considered.
Overview

As environmental protection has progressed from end-of-pipe controls on emissions to pollution prevention, new challenges have arisen. Pollution prevention seeks to reduce harm to the environment and human health through changes in manufacturing processes. An understanding of the health and environmental risks posed by alternative pollution prevention strategies is crucial in decision making. Nowhere is this more apparent than with the foremost pollution prevention technique, substitution of a toxic chemical with a non-toxic or less toxic chemical alternative or technology.

With the advent of the Toxic Use Reduction Act (TURA) in Massachusetts, companies have additional incentives to undertake chemical substitution. TURA\(^1\) requires that firms prepare annual reports of their use of listed toxic chemicals and their progress in reducing by-products and emissions. Beginning in 1994 each firm must prepare a toxics use reduction (TUR) plan that identifies programs and goals for reducing generation of toxic by-products through the adoption of various TUR techniques. TUR techniques, as defined by the Act, are input substitution, product reformulation, production unit redesign or modification, improved operation and maintenance, and recycling that is integral to the production process. Chemical substitution is very attractive to firms under the TUR approach because it achieves 100% reduction in use of a listed chemical while other approaches lead to smaller reductions. In addition, because the list of target chemicals for TURA is made up of lists from other regulatory programs (such as the Toxics Release Inventory (TRI) and the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA or Superfund)) a substitution will allow a company to avoid compliance concerns with these laws as well.

As many forces converge to encourage substitution for toxic chemicals in production processes, it is imperative that substitution decisions remember the goal of TUR -- reducing risk to human health and the environment\(^2\). Risks may take many forms. An application of a chemical may produce acute or chronic health risks to workers or the public. It may cause safety risks, such as fire or explosion. It may be associated with environmental risks including health risks to some ecosystem populations, global warming potential, or ozone depleting potential. Only through explicit consideration of risk, a product of the hazard(s) posed by a substance and exposure of the relevant receptor, can the risks of alternative chemicals be judged and risk reducing substitution decisions made.

\(^1\)All discussions of the TUR strategy are drawn from MA TURA, one of the earliest and most ambitious TUR laws (hereinafter MA TURA) as found in Commonwealth of Massachusetts H.6161, General Laws Chapter 211, June, 1989.

\(^2\)MA TURA § 2
This project examines the role of risk in companies decision-making about chemical substitution. After evaluation of the needs of companies, and the current models available for chemical substitution, a proposal for a substitution decision making process is outlined.

What is Chemical Substitution?

Chemical substitution in pollution prevention is, quite simply, the replacement of one chemical in a process step with another. The approaches to pollution prevention and TUR, other than chemical substitution, tend to focus on reducing exposure to a chemical currently in use. Substitution may lead to exposure to a new and different chemical. Chemical substitution is of special concern in TUR because it has the potential to increase risks if a decision is not made carefully. Substitution under TURA is guided by the list of toxic chemicals. It is implicitly assumed that risk will be reduced by substituting a material off the list for one on the list. Yet the lists of toxic chemicals used in pollution prevention and TURA have a very inconsistent and highly variable basis in toxicology or risk. In addition, the chemicals on the lists often reflect a preoccupation with potential human health effects with little attention given to environmental and ecological hazards.

The science of toxicology has as its basic tenet that all chemicals have the potential to be toxic, what differs between chemicals is the dose at which they are toxic. For example, an adult human would have to eat about 1/2 pound of table salt in a few hours to achieve a fatal dose while only about 1/4 of a teaspoon of strychnine would be fatal. In addition, some chemicals have special hazardous properties such as the ability to contribute to global warming or stratospheric ozone depletion. A focus on toxicity may mean that other hazardous properties of chemicals, such as flammability and explosiveness, may not be considered in a “list-based” approach to chemical substitution.

Risk analysis, broadly defined, is a method for organizing and using scientific information about uncertain events. It has been used in engineering and public health for many years. Chemical risk analysis evaluates risk by combining the intrinsic hazard of the material with the level of exposure. Chemicals may have several hazardous properties including

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4 Laden, F. and Gray, G. M., supra

flammability, carcinogenic potential, or neurotoxic effects. For each of these hazards there is an exposure-response relationship which describes how likely the effect is for a given level of exposure. Because chemicals differ in the exposure level at which toxicity occurs it is imperative to consider both hazard and exposure when evaluating risks of chemical use. For example, even if a firm substitutes a less toxic chemical, for example one with a cancer potency only 1/3 that of the original, if the new material is more volatile and exposure to workers increases, or is less efficient and requires greater use of the substitute chemical, the risk could actually increase.

It is clear that potential risks, to workers, the public, and the environment, must be an explicit consideration in chemical substitution decisions.

I. How Are Chemical Substitution Decisions Currently Made?

To understand how companies are making chemical decisions under the Massachusetts Toxics Use Reduction Act (MA TURA) a series of interviews were conducted with representatives of Massachusetts companies. The sample was small and not randomized. Companies that had recently made chemical substitution decisions, identified with the help of the Massachusetts Toxics Use Reduction Institute, were the focus. Representatives from five Massachusetts firms were interviewed. These firms were Lampin Corporation, Hyde Manufacturing Company, M/A COM, Printed Circuit Corporation, and Polaroid Corporation. The companies range in size from about thirty to many thousand employees, and all had recently made chemical substitution in a manufacturing process. The motivation for substitution ranged from regulatory concerns (i.e., reducing use of chlorofluorocarbons) to company wide pollution prevention efforts. The purpose of the interviews was to learn how different companies approach pollution prevention and TUR and to characterize the substitution process employed by each firm. Of primary interest was the role that risk played (or did not play) in substitution decisions.

The goal of each interview was to understand the specific substitution decision making processes used by a company and the rationale for the process. The major objectives of the

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6Companies Interviewed:

**Lampin Corporation**, Uxbridge, MA
manufacturer of precision metal-stamped components

**Hyde Manufacturing Company**, Southbridge, MA
manufacturer of metal-stamped hand tools

**M/A COM**, Lowell, MA
manufacturer of diodes, semi-conductors and integrated micro circuits

**Printed Circuit Corporation**, Woburn, MA
large quantity manufacturer of custom made printed circuit boards

**Polaroid Corporation**, Cambridge, MA
manufacturer of instant image-recording products
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interview were to identify (1) the sources that companies use to identify potential substitutes; (2) which sources were considered most useful; and (3) how companies choose among alternative chemicals. This meant understanding the criteria that are used to evaluate each alternative and how the criteria are weighed. Finally, the role of risk, to workers’ health and safety, to the public, and to the environment, in the decision process was evaluated.

The methods by which these companies make their substitution decisions range from ad hoc to methods that are defined, structured, and documented. The less sophisticated substitution decision making processes were seen in the smaller sized companies. As might be expected, these firms have many fewer resources to devote to a substitution decision and the judgment is usually made by a single person. In one case, it is the President who weighs the attributes of concern and makes the substitute decision, while at another company the decisions are made by the Environmental Engineer. Another important fact is that the smaller companies, which in general use fewer chemicals, generally see their recent substitution as a one time effort to solve a particular problem. This is in stark contrast to the larger firms which use the idea of continuous improvement to guide pollution prevention activities.

The more elaborate decision making systems are found in the comparatively larger firms with many more resources, often including a environmental, health, and safety department. At these firms, teams and task forces made up of people from many disciplines are involved in the identification and analysis of substitution choices. One firm’s system also includes the research and development of new processes and materials. In many large firms teamwork is a long established approach to making other business decisions. This familiarity may explain why larger firms use a group approach to chemical substitution decisions. In addition, it seems that the larger firms have devoted more effort to decision making systems because the corporate culture now stresses continuous improvement toward environmental goals.

Identifying companies’ sources of information on the relative merits of alternative chemicals was a focus of the company interviews. It was found that most companies use an array of sources to help identify potential chemical substitutes. Smaller companies tend to rely on resources external to their firms, especially vendors, as well as the Massachusetts Toxics Use Reduction Institute at the University of Massachusetts, Lowell (TURI), the Massachusetts Office of Technology Assistance (OTA), and “word of mouth” from industry networks and conferences.

7For example, it its Annual Report on the Environment the statement from Polaroid CEO I. MacAllister Booth states that continuous improvement in environmental performance is a key commitment of the company.
(like those conducted by the Merrimack Valley Business Environment Network). Overall, vendors seem to be the major source of information for the smaller firms.

Larger firms, on the other hand, rely primarily on resources from within their own companies. Substitutes may be identified by the company’s research division, from the scientific or engineering literature, or in the more informal ways used by small firms. Evaluation of alternatives is often quite structured. For instance, M/A COM has a pollution prevention task team at each of its facilities. These teams consist of manufacturing, and design development engineers, accountants, environmental managers, health and safety specialists, and others. When the company is faced with searching for a substitute, each team member shares his or her ideas for alternatives. These internally generated ideas are the foundation for the remainder of the substitution decision making process and for future decisions. The substitution options are then evaluated by a structured protocol developed by the company's Environmental Engineering group. M/A COM is currently generating a substitution options book to be used internally which lists materials that have been characterized by them as most desirable.

While small firms rely primarily on external resources and large firms rely on internal ones, all firms use both types of resources. For instance, at one small firm employees are encouraged to share their substitute ideas and continuous improvement suggestions, while at one large firm it is not unusual to turn to outside experts for toxicological advice. It was clear that all five firms interviewed thought OTA and TURI were very useful sources. In fact, OTA and TURI were described as "very important", “knowledgeable”, and "process specific" and were appreciated for giving industry representatives confidence in their decision making processes. However, one interviewee believed that these groups were no more sophisticated than himself and thus were not very useful to him. No other sources stood out as exceptional resources for any of these companies.

Key to understanding how firms make substitution decisions is understanding what attributes of alternative chemicals are considered important. Substitute attributes considered include cost, performance, regulatory compliance, liability and health risks. Not all firms considered the same attributes. The weighing of the different attributes (e.g., does it make sense to use a chemical with lower performance for the sake of regulatory compliance) differs among companies. For some, one attribute, cost, dominates the decision. Others attempt to generate explicit weighting systems for the different factors, including different health and safety endpoints. It was not clear if these explicit weighting systems had ever been fully utilized in
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making a substitution decision. This may have been because a complex, data intensive protocol is considered unnecessary when one substitute seems clearly superior.

Interestingly, each company surveyed had already been involved with pollution prevention or substitution when TURA was enacted, with the exception of one firm which initiated its substitution efforts as a direct response to TURA and The Clean Water Act. Another company had established its Toxic Use and Waste Reduction Program, which evaluates each material in use and those under consideration for use for its potential impact on the environment, taking into account its chemical and physical properties and toxic characteristics, well before the Massachusetts Toxic Use Reduction Act was enacted.

II. Decision-Making Schemes

Several proposals have been put forward to aid in chemical substitution decisions but the role of risk analysis in evaluating chemical substitution decisions has received relatively little attention to date. It has been recognized that substitution may replace a risk with a similar risk, change the form of risks (i.e. risk of neurotoxicity to fire risk) or lead to real risk reduction 8.

An ideal scheme for the consideration of risk in chemical substitution would use information on the toxic potential of alternative materials along with information about the exposure expected with a specific application, to explicitly identify the lower risk alternatives. In addition the scheme would provide an understanding of the magnitude of all relevant environmental, health, and safety risks. The scheme should be flexible enough to evaluate new chemistry as it is developed and should provide information which will allow continuous improvement to be monitored.

However, it is clear that risk is only one of several important attributes that must be considered in a substitution decision. The importance of different factors, such as cost, performance, reliability, and risk differs by firm, by application, and by chemical. Therefore, a decision making scheme should recognize that a substitution decision has many attributes and no prescriptive “one size fits all” approach can be developed for the many circumstances of chemical use.

In this section several approaches to chemical substitution, identified from the literature and regulatory agencies, are outlined. Some of the schemes acknowledge risk and attempt to objectively evaluate the hazards of alternative chemicals while others are oriented toward choosing more desirable alternative chemicals.

Generic Classification System

The goal of the Generic Classification System is to help users make solvent substitution decisions by developing general categories of chemicals. The scheme sets up eight categories of solvents based on physical properties and environmental effects. Physical properties include volatility, flash point, and the presence or absence of different halogen atoms. The environmental effects focus on ozone depleting potential and global warming potential with some consideration of toxicity. The scheme does recognize that there are risk tradeoffs in substitution, for example flammability versus global warming potential, but there is no explicit or quantitative consideration of risk. Instead, regulatory attention (such as presence on the 1990 CAAA list of hazardous air pollutants) is used as a surrogate for hazard.

Advantages of the generic classification system are several. First, the development of a structured framework with clear rules based on physical-chemical properties means that the approach can be used with existing and new materials. The system attempts to make companies think prospectively about the potential impact of a substitution decision. The system also recognizes, though does not address, how to deal with the potential toxicity of less tested alternative solvents.

On the other hand, there are several drawbacks that make the generic classification system insufficient for informed substitution decision-making. First, it focuses on solvents, with categories based on generic properties of solvents which will not be applicable to other chemistries. Other than mention of compliance issues, the only environmental, health, or safety factors explicitly considered are global warming and ozone depleting potentials. Although it acknowledges some of the many risk/risk tradeoffs in substitution, by ignoring many types of health and environmental risk the generic method does not make firms face up to the many tradeoffs in a substitution decision. It also does not allow identification of major sources of exposure and risk. Finally, since it does not encourage explicit consideration of changes in exposure potential or hazard it may not lead to risk reduction.

Tellus Decision Framework

The Tellus Institute, under contract to the Massachusetts Toxics Use Reduction Institute (TURI), developed a framework for chemical substitution\textsuperscript{10}. The goal of the system is a decision framework to assess substitutes on technical, economic, regulatory, and institutional considerations. The process primarily aids in the identification of potentially useful substitutes.

The proposed system sets up a sequential framework which is entered when certain trigger mechanisms are invoked. The procedure then begins with a process to examine the function of the current chemical. Users are encouraged to carefully evaluate how the chemical is used in each process or product. Identification of substitutes focuses on finding technically proven chemical or non-chemical methods through vendors, trade associations, technical assistance programs and other sources. Economic feasibility and production effects are considered next. Finally, environmental health and safety are addressed by focusing on compliance and considering environmental, consumer, and occupational health. Each level of the framework contains yes/no decisions which either lead further in the framework (yes) or remove a substitute from consideration (no).

The proposed approach has the strong advantage that it encourages a structured approach to substitution. In addition, it considers the multiple important attributes of a substitution decision. At times it is a bit too complex, for example for economic feasibility it suggests the use of full cost accounting and for EH&S suggests a lifecycle analysis. However, this structured approach to a complicated problem is a step forward and, perhaps, it is better to be too ambitious than too simple. Finally, the framework does recognize the potential health and environmental risks of substitute chemicals and technologies although it does not go the extra step of discussing an approach to deal with this problem.

Perhaps the largest impediment to real world use of this framework is its highly prescriptive nature. Decision points are evaluated according to strict rules. For instance, the framework asks if a substitute is economically feasible without clear definition of this broad and highly subjective company-specific test. If the answer is no it suggests rejecting the substitute. However, it may well be that a firm would want to use a less economical alternative for other reasons or it may be that an economically viable alternative is suboptimal on another attribute. The substitution decision process needs flexibility. Another drawback to the framework is the lack of explicit guidance for evaluating health, safety, and environmental risks. A focus on

compliance leads right back to the problem of substituting well studied compounds for those with unknown toxic potential.

**Lifecycle Inventory and Tradeoff Analysis Method**

The Lifecycle Inventory and Tradeoff Analysis Method\(^\text{11}\), created by the Source Reduction Research Partnership for the Metropolitan Water District of Southern California and Environmental Defense Fund, involves a detailed and methodological comparative analysis, with results that are not absolute, but provide insight to the local and global impacts associated with a given source reduction option.

The Lifecycle Inventory and Tradeoff Analysis Method identifies categories of impact (e.g., global warming, air quality), assesses each to a limited degree, and weighs the impacts relative to one another.

The Method follows three steps:

1) Energy consumption, material inputs, and material outputs including environmental emissions, are quantified for each alternative on both the local and global level. This step develops the lifecycle inventory.

2) Significant impacts due to energy consumption, material inputs, and material outputs are identified.

3) Impacts are rated and tradeoff comparisons made.

An Impact Analysis Matrix is used for making the trade off comparisons. The matrix’s rows define environmental risk areas like land disposal, water quality, and ozone depleting potential. Its columns contain impacting parameters like energy inputs and atmospheric emissions. Unweighted scores (+1,0,-1) are assigned to the impact categories to indicate the strengths of the proposed alternative compared with the base case. This method encourages the use of a multidisciplined group of experts to review the scores in the matrix and to scrutinize each score until a consensus among group members is reached.

The creators of the Lifecycle Inventory and Tradeoff Analysis Method stress that alternatives that appear favorable when examined at the local use level can sometimes reveal unanticipated impacts when examined from a broader perspective, like impacts associated with

manufacturing and raw materials production. When assessing alternatives it is important to delineate these impacts and to judge their relative importance. This judgment requires a methodical comparative analysis. Unlike current lifecycle assessments, this method carries alternative assessments out an additional step by measuring impacts on the environment or human health. Most current lifecycle assessments are limited to "inventorying" inputs and outputs, and fail to examine actual impacts and assign relative weights to those impacts.

The advantages of the Lifecycle Inventory and Tradeoff Analysis Method include its explicit acknowledgment of impacts beyond facility level use of a material. It urges users to consider systematically the environmental and public health impacts throughout the lifecycle of alternative technologies. The major drawback is that the method does not explicitly address exposure or risk. In addition, the lack of available data for many stages of a lifecycle inventory leaves the analysis dependent on many critical assumptions.

Several other schemes have been described in the literature\(^\text{12}\). Most focus on methods for identifying potential substitute chemicals. All fail to explicitly consider exposure and toxicity potential of alternative chemicals but instead rely on regulatory compliance as an indicator of risk reduction. Two firms interviewed for this project, Polaroid and M/A Com have developed internal substitution schemes\(^\text{13}\). Both involve consideration of the health and safety hazards of alternative chemicals. Both schemes are quite resource intensive and in one case it was not clear that the protocol has ever been fully applied to a substitution decision.

**Conclusion**

Explicit consideration of risk, that is the combination of hazard and exposure, is not a feature of any current proposals for chemical substitution decision making. This may be because the limitations of data and models are believed to present too much uncertainty to make comparisons meaningful. It may be because many believe that alternative chemicals are likely to be less toxic because they are not yet under regulatory scrutiny. Finally, it may be that current

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\(^{13}\)Hawes, Tim, Manager of Compliance, Polaroid Corporation, Personal Interview, March 4, 1994; Surette, Edward, Environmental Engineering Manager, M/A-COM, Personal Interview, February 16, 1994.
regulatory procedures provide no incentive for evaluating risk because it is unnecessary for regulatory compliance.

Few of the existing schemes are flexible, allowing a firm to tailor a decision to suit the particular needs of its process. The U.S. EPA’s Use Cluster Scoring System, currently under development, is a step in this direction. Clearly, there is no reason to believe that a single decision making scheme can be prescribed for all uses of chemicals. Instead, a firm must weigh competing attributes, such as cost and performance, as well as competing risks, such as human health risk, safety risks or ecological risks. What is needed, then, is not a highly regimented checklist type approach to substitution but rather the development of a decision making process which explicitly considers the health, safety, and ecological risks of alternative chemicals as inputs to the substitution decision.

III. The Chemical Substitution Tree

It is clear that a framework is needed which encourages firms to evaluate the health and environmental risks of chemical substitutes. The chemical substitution tree (CST) is presented as a first step in the development of tools to help companies in pollution prevention and chemical substitution decisions. The tree provides a structure for a sequential process of evaluating potential exposures due to use of a chemical, potential hazards associated with a given chemical, and the risk that is due to the combination of exposure and hazard.

However, it is evident that risk is only one of several important attributes that must be considered in a company’s substitution decision (Figure 1). The importance of different factors, such as cost, performance, reliability, and risk differs by firm, by application, and by chemical. Therefore, a chemical substitution decision-making scheme should recognize that a substitution decision has many factors and no prescriptive “one size fits all” approach can be developed for the many circumstances of chemical use. Currently, the health and environmental risks of substitute chemicals are not systematically assessed. The chemical substitution tree lays out a process which companies considering chemical substitution will be encouraged to implement. This process will make consideration of the exposure and hazard of alternative chemicals explicit and will help ensure that pollution prevention decisions truly reduce risk.
The Framework

The tree is designed for comparison of a potential substitute chemical with the base case chemical. The tree can also be used to evaluate new technologies and other pollution prevention options. It sets up a sequential process in which potential exposures and hazardous properties of the substitute chemical are evaluated and qualitatively or quantitatively compared to the base case. The goal is to ensure that major sources of potential risk to the environment and human health are considered. The use of comparisons should make the evaluation easier. It is not necessary to get the absolute right answer, only to know which alternative is superior for each important attribute.

The tree structure is a compromise between completeness and tractability for any given decision context. The tree structure is very general and can be “grown” or “pruned” according to the decision at hand and the resources of a particular firm. For illustrative purposes, the tree described here (Figure 2) focuses on risks from the use and disposal of two alternative chemicals. Ideally, the tree would be used to evaluate sources of risk for the entire lifecycle of alternative chemicals and technologies including changes in energy use for the alternative chemicals. It is clear that consideration of changes in
Figure 2 - The Chemical Substitution Tree
energy use (and concomitant risks\textsuperscript{14}) may be very influential in evaluating chemical alternatives\textsuperscript{15}. In any substitution analysis as complete a tree as possible should be evaluated.

The potential risks must be considered in the substitution decision along with cost, performance (isopropyl alcohol is inferior to trichloroethylene in many applications), and other factors. An advantage of the CST is that it allows identification of sources of potential risks and may point to risk mitigation procedures. Decreasing or preventing worker contact with trichloroethylene or its vapors, identified as a potential source of risk in the CST, may mean that, given the many other factors, it is the superior material for a degreasing application.

Each path through the tree (Figure 2) illustrates a particular exposure situation and type of toxicity. The framework illustrated is concerned with potential exposures during the intended use of the chemical and the potential exposures associated with disposal of waste. Exposures associated with use include handling of the material (including spills and accidents), those related to the normal use of the compound, and anticipated emissions to air, water, and land. Potential exposures during disposal arise from transportation and handling of the waste and from the method of disposal (\textit{i.e.}, landfill, incineration). The goal of this portion of the tree is to identify potential sources of human and environmental exposure during the use and disposal of the base case and alternative chemical.

Under conditions of normal use there may be exposure to the environment, the public, and workers. Emissions and spills are the primary sources of exposure for the environment and the public. Workers may be exposed through normal use of the material, through handling and transport, as well as through spills. The main routes of exposure for the public are emissions and spills. Similar potential exposures are generated during disposal of the chemical.

Estimation of exposure levels may be much easier for the chemical already in use, the base-case chemical. Information from industrial hygiene monitoring or modeling of workplace exposures can be used. Records on occurrence and magnitudes of accidents and spills can be consulted. Public exposure from emissions can be measured or modeled using available information. Judging potential exposures for the chemical not yet in use will be more difficult.


\textsuperscript{15}CA/EDF Study, \textit{supra}
Comparison with similar compounds in similar processes may allow rough estimation of exposure levels. Various models have been proposed to estimate potential workplace exposure to solvents based on physical-chemical properties\textsuperscript{16}. In many cases, the expert judgment of industrial hygienists may be an important source of information\textsuperscript{17}.

In each case the potential hazards must be assessed in conjunction with foreseeable exposures. This is the purpose of the hazard portion of the tree.

Potential hazards are evaluated, relative to the base case, for the potential exposures to the environment, workers, and the public. With environmental exposures there are concerns for both large scale (including global) effects and local effects. Large-scale effects might include global warming potential, ozone depleting potential, or long range transport of hazardous pollutants. Possible human health risks are evaluated for both workers and the general public. In addition, exposures to the public are evaluated as both consumers of a product (when applicable) and as the community potentially exposed to emissions of a chemical. Endpoints of concern include safety risks, such as flammability, explosivity, and physical hazards, as well as both acute and chronic toxicity.

Some potential measures for the various endpoints are listed in Table 1. Some hazard information will be available as part of a chemical’s material safety data sheet (MSDS). There are several other sources of information on potential toxicity measures available, many of which are now on-line. On-line sources include the U.S. EPA’s Integrated Risk Information System (IRIS), and the National Library of Medicine’s TOXNET. IRIS includes data on chronic toxicity, including reference doses and carcinogenicity assessments, as well as measures of acute toxicity such as one-day or ten-day drinking water health advisories. Resources on TOXNET include: the Hazardous Substances Data Bank (HSDB) which contains toxicological information on over 4000 chemicals; the Registry of Toxic Effects of Chemical Substances (RTECS) which contains available acute and chronic toxicity data on over 100,000 chemicals; the Chemical Carcinogenesis Research Information System (CCRIS) which contains information on mutagenicity and carcinogenicity of many chemicals; GENE-TOX, which contains genetic toxicology data on over 3000 chemicals; and Developmental and Reproductive Toxicology (DART) which is a bibliographic database with information on teratology and developmental toxicology studies.


For example, replacing trichloroethylene with isopropyl alcohol in a degreasing operation might lead to an ↑ at the end of the use/worker/chronic toxicity branch because trichloroethylene (the base case) raises concerns about carcinogenicity that isopropyl alcohol does not, so the substitute is considered superior. On the other hand, at the end of the use/worker/safety branch there might be a ↓ because the flammability of isopropyl alcohol makes it less attractive than the base case.

<table>
<thead>
<tr>
<th>Endpoint</th>
<th>Possible Measures</th>
</tr>
</thead>
<tbody>
<tr>
<td>global environmental hazard</td>
<td>global warming potential (GWP) or ozone depleting potential (ODP)</td>
</tr>
<tr>
<td>local environmental hazard</td>
<td>aquatic or terrestrial organism predicted no effect concentration (PNEC)</td>
</tr>
<tr>
<td>worker and public safety</td>
<td>flammability (e.g., flash point), explosivity, corrosiveness, irritation, EPA RCRA Reportable Quantity (RQ)</td>
</tr>
<tr>
<td>worker and public chronic toxicity</td>
<td>reference dose (RfD (18)) or acceptable daily intake (ADI), cancer slope factor for suspected carcinogens; occupational threshold limit value (TLV)</td>
</tr>
<tr>
<td>worker and public acute toxicity</td>
<td>oral or inhalation LD&lt;sub&gt;50&lt;/sub&gt;, dermal or ocular irritation, EPA drinking water health advisory one-day or ten-day acute toxicity levels, EPA Threshold Planning Quantity</td>
</tr>
</tbody>
</table>

Table 1. Potential Measures for Various Endpoints in the Chemical Substitution Tree

A major problem that will arise as firms implement this protocol is that very little data is likely to be available for chemicals not on the list of toxic compounds. Many believe that the lists used in TUR are dominated by well studied compounds and that if chemicals off the list were subject to the same scrutiny they would also be considered of concern. Several methods are available for dealing with the asymmetry of hazard information. The hazardous potential of untested compounds can be roughly estimated by quantitative structure activity relationships.
(QSAR) in many cases\textsuperscript{18}. Methods have been developed to derive provisional RfD’s from acute LD\textsubscript{50}s\textsuperscript{19}. Similarly, a combination of QSAR and knowledge of acute toxicity can provide very rough estimates of carcinogenic potency\textsuperscript{20}. Because the use of this information would be internal to a firm there might be a willingness to experiment with nontraditional methods of estimating toxic hazard. In addition, the demand for such information may increase both the generation of scientific data and the development of methods to estimate hazard with limited information.

It is key that the final evaluation rely on both the potential for exposure and the hazard posed by a substitute. It may be that cases will arise in which a substitute with much higher exposure potential is desirable because its toxicity is so much lower than the base case.

\textit{Output of the Process}

For each endpoint of concern the potential exposure is combined with an estimate of the relative hazard of the substitute chemical to yield a qualitative judgment of the direction of risk. For example, a substitute for a chlorofluorocarbon might have higher emissions during use but when combined with a much lower estimate of global warming potential (GWP) would rate a $\Box$ at the end of the use/environment/global branch of the tree because overall the substitute’s global environmental risk is lower than the base case chemical. The final output of the substitution tree evaluation is a qualitative evaluation of the relative risks of the two alternatives that allows an understanding of situations in which the substitute chemical is expected to pose lesser risks, greater risks, or similar risks, to the chemical currently in use. The ultimate decision of whether or not to substitute, or which substitute to use, must weigh additional attributes of each material but the substitution tree ensures that the environmental, health, and safety risks posed by alternative chemicals are explicitly considered.

The process of evaluating the environmental, health, and safety risks of alternative chemicals will force firms to make these attributes an explicit part of a substitution decision. How the attributes are weighed (global warming potential versus the risk of fire, for example) will be specific to each firm and each decision. However, if this protocol were to become common practice as part of corporate environmental decision making, like “benchmarking” and


the spread of Total Quality Environmental Management (TQEM), it would likely have a strong impact on substitution decisions. It is imperative that human health and environmental risk play a key role in chemical substitution for pollution prevention. Making the regulatory community and the public more aware of the tradeoffs and difficult choices in these decisions might also help to raise the general level of discussion around pollution prevention and risk reduction.

A further advantage of the thorough evaluation of potential risks is that opportunities for risk reduction may be identified. For example, if a substitute chemical is found to be generally safer than the base case material but concerns about its acute toxicity in case of accidental spills are identified in the substitution analysis, steps may be taken to minimize spill potential thus making the substitute even more attractive. In addition, as substitution analysis becomes more widespread obvious data gaps will become apparent stimulating work to better characterize the hazards of alternative chemicals. Finally, explicit evaluation of sources of risk may mean that other pollution prevention opportunities, focused on exposure reduction, will become more attractive and substitution will not be necessary.

**Conclusion**

To achieve the goal of pollution prevention and toxics use reduction it is clear that risk must be considered in chemical substitution decisions. Toxicology reminds us that all compounds can be toxic at some dose. The toxic potential of substitute chemicals cannot be ignored. It is also apparent that reliance on regulatory compliance, avoiding substances on lists of toxic chemicals, is insufficient. The lists have little consistent risk or toxicological basis and frequently have little concern with ecological or environmental effects. In many cases exposure is the key. For it is the combination of exposure and toxicity that determines risk. For this reason, designation as toxic is not enough to understand the risk posed by a chemical, just as absence from a list of hazardous substance does not guarantee safety. At the same time, knowledge of exposure to a chemical without knowledge of its toxicity is insufficient information to understand risk. It is the combination of exposure and hazard, risk, that is the appropriate metric for analyzing and measuring progress in pollution prevention.

The chemical substitution tree was developed to encourage companies to think about sources of exposure and risk. It is a forward looking process which allows companies to identify and avoid future problems. Through analysis of environmental and human health and safety risks the CST will encourage decisions that lead to real risk reduction. In addition, by identifying areas of potentially high risk the process can help companies find opportunities for additional risk reduction and continuous improvement.
Companies should be encouraged to implement the CST approach. When possible, the results and documentation of the process should be shared. There is a need to demonstrate the process and identify possible trouble spots. One potential problem is the availability of toxicological information on many substitutes. A great help could be provided by state or federal groups with scientific expertise acting as clearinghouses for information on the hazards of substitutes. As use of risk based chemical substitution becomes more wide spread it means that reliance on admittedly scientifically indefensible lists of toxic chemicals may be reduced. It may well be that large risk reduction can be achieved by substitution within the list, an option that few companies will attempt today. We will make progress toward protecting human and environmental health and safety in pollution prevention by putting scientific knowledge and the tools of risk analysis to work.