# TOXICS RELEASE INVENTORY
# ENVIRONMENTAL INDICATORS METHODOLOGY

Prepared for:

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September 23, 1992

DRAFT REPORT

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UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

March 29, 1993

Dear Colleague:

Please find attached a copy of the draft report Toxics Release Inventory Environmental Indicators Methodology. Earlier I had indicated to you that you would not be sent a copy of the draft as the final version was to be completed in the near future. Due to unforseen circumstances it has not been possible to complete the final version in the time frame originally envisioned. Therefore, I am sending you a copy of the draft as many of you expressed an interest in applying the methodology to issues currently at hand.

I hope you find the report useful. If any assistance is required in its interpretation please feel free to contact me at 202-260-1567, or by writing to the address above, including the mail stop TS-779. If you feel a final copy would be needed in the future you may request a copy.

Sincerely,

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**Acknowledgements**

This draft report was prepared by Abt Associates under the guidance of the TRI Environmental Indicators Work Group. Work Group members include:

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# EXECUTIVE SUMMARY

In 1989, the Environmental Protection Agency (EPA) initiated an effort to focus resources on regulatory or other programs that have the greatest potential to achieve reductions in health or environmental risks. As part of this effort, the Agency began to explore ways to evaluate its successes in reducing risks, an effort which includes the development of indicators of environmental progress.

The Office of Pollution Prevention and Toxics (OPPT) is in the process of developing indicators of the impacts of chemical emissions on human health and the environment over time. The indicators being developed by OPPT are based on existing data sources that reflect multimedia trends in environmental contaminant releases, and designed to be flexible enough to incorporate additional chemicals and sources as more information becomes available.

The database selected as the basis for OPPT's environmental indicators is the Toxics Release Inventory (TRI), which contains annual reports documenting multimedia environmental releases and off-site transfers for over 300 toxic chemicals from U.S. manufacturing facilities and which are of concern to the Agency[1]. Although the TRI database does not capture all chemicals or industry sectors of concern to both OPPT and the Agency as a whole, the database is the Agency's single best source of consistently reported emissions data.

The TRI Environmental Indicators may eventually consist of a set of four indicators, chronic and acute human health impacts, and chronic and acute ecological impacts. The focus of this report is the development of indicators of chronic effects to human health and to aquatic life. The development of corresponding acute effects indicators is not feasible now, since key data to support such indicators are not available. To appropriately evaluate potential acute effects, one would need to know the distribution of releases over time (peak release data), and these data are not currently reported to TRI.

The ultimate goal of the indicator effort is to devise a measure that reflects the impacts of chemical releases and transfers, which can be used to assess progress in reducing these impacts over time. The indicator methodology should be comprehensible, replicable, and easily adaptable to a computer program. The methodology should also be sufficiently flexible to facilitate separate analyses of the relative contribution of indicator components, such as release media, industry sectors, chemicals, and geographic areas. The methodology should also have provisions that either provide for uncertainty or provide alternatives when

[1]The TRI is mandated by the Superfund Amendment Reauthorization Act (SARA) Title III Section 313.

data are unavailable. The method should be sufficiently flexible to permit updates as new chemicals/industries are added to TRI. Finally, all assumptions on which the indicator is based should be easily identifiable and understood.

This report explains how the proposed TRI Environmental Indicators are constructed, and includes discussions of the conceptual methodology, data sources, and computational approach. The proposed indicators are based on risk-related scores, and the report discusses the similarities and distinctions between the risk-based approach of the indicators and conventional risk assessments.

In developing the proposed indicators, many approaches to assessing and ranking the potential risk of chemicals were reviewed. Numerous techniques to score the relative significance of TRI chemicals and facilities have been and continue to be developed. One objective of this report is to explain the indicator to a variety of agencies and groups that may wish to use it or to adapt the indicators or the methodologies to their own needs. A related objective is to describe the benefits of the proposed approach to the indicator in terms of flexibility, power as an analytic tool, and usefulness as a policy tool.

## GENERAL DESCRIPTION OF THE TRI ENVIRONMENTAL INDICATORS

The objective of the indicator methodology presented in this report is to construct a unitless value that is related to the overall impacts of releases and transfers of all included TRI chemicals by all facilities to each environmental medium at a given point in time. The indicators are planned to be calculated each year based on the most current TRI data, and compared to previous years' indicator values. One of the early years of TRI reporting, e.g. 1989 , would be selected as a "base year" and later years' indicator values compared to it. For the base year, the unitless score would be normalized to a round number such as 10,000; subsequent years' data would be normalized by the same factor to provide a relative comparison. This will allow assessment of the changes in estimated impacts of TRI releases and transfers from year to year.

Four components are generally used to compute each indicator (e.g. for human health chronic impacts). These are:

- the quantity of a chemical released or transferred,
- a toxicity weight,
- a weight reflecting the size of the potentially exposed population, and
- an exposure potential weight.

Separate assessments are made for each unique combination of a chemical, facility, and release medium. For each of these releases or transfers, one develops an indicator "element": a unitless value proportional to the potential impact of each specific release or transfer. The value for each TRI indicator is simply the sum of all the indicator elements.



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It must be emphasized that the TRI Environmental Indicator methodology is not intended to be a quantitative risk assessment and does not calculate risk estimates. The proposed methodology utilizes some of the tools often applied in quantitative assessments, but in a relative way. The TRI indicator is by its nature only intended to reflect the direction and the general magnitude of the change in releases over time, scaled by factors (toxicity, exposure potential, receptor population size) that relate to potential risk. As such, this indicator value has only relative rather than absolute meaning; it can only be used in comparisons to other values at different points in time, or in identifying the relative size of contributing factors.

**Human Health Chronic Indicator**

Each element of the Human Health Chronic Indicator (which is facility-chemical-medium-specific) consists of three components: toxicity, exposure (which includes release size), and the size of the exposed population. Components are multiplied to calculate the element value. It must be reiterated that an element value is not an absolutely meaningful measure of risk associated with the facility. These values are useful as an approximate measure that is comparable to approximate measures for other facilities calculated using the same methods, to identify relative significance.

The current proposal is focused on general populations: individuals, particularly highly exposed individuals, are not the focus of the indicator. Additional indicators based upon highly exposed or sensitive subpopulations may be developed in the future.

**Ecological Chronic Indicator**

For the Ecological (aquatic life) Chronic Indicator, the elements are developed by combining aquatic toxicity and exposure components for each facility, each chemical, and each medium. As with the human health chronic indicator, each component contributes multiplicatively to the overall magnitude of the element value. For the Ecological Chronic indicator, the population component is not utilized, since the size of the exposed population is typically not known, and because of the difficulty in relating impacts to ecological systems with many exposed populations of organisms.

## SELECTION OF CHEMICALS TO INCLUDE IN THE INDICATORS

In order to be as inclusive as possible and still maintain computational tractability, a large subset of TRI chemicals should be included in the indicator. Factors considered for determining whether to include a chemical include the availability of necessary data to compute elements , and the magnitude of emissions. The following criteria are proposed to exclude TRI chemicals from the indicator:

- Exclude chemicals with no reports in 1989 (56 chemicals) or only reports listing zero releases and transfers (17 chemicals, for a total of 73);

- Exclude chemicals with no readily available EPA-reviewed toxicity data (the number of chemicals is not currently known, as toxicity data reviews have not been completed).
- Possibly exclude chemicals with total releases to each medium below some threshold, e.g. 1000 lb (about 14 chemicals). The initial list of chemicals meeting this criterion is being reviewed to identify (and delete) ones which may exhibit toxic effects at low concentrations.

## METHODS FOR ADJUSTING EMISSIONS FOR TOXICITY AND EXPOSURE

To construct indicator elements that are related to risk, the emissions must be adjusted in a manner that reflects the risks associated with each media-specific release or transfer of each chemical. The risk potentially posed by a chemical emission depends on the inherent toxicity of the chemical, the environmental fate and transport of the chemical in the medium to which it is released, the degree of contact between the contaminated medium and the human or ecological receptors, and the size of exposed populations. Differences in toxicity among chemicals, as well as differences in environmental fate and in the size and characteristics of populations potentially exposed influence the relative contribution each emission makes to each indicator. Transfers to offsite locations such as sewage treatment plants (POTWs) require an additional estimate of the impact of treatment technology on the emissions.

In order to incorporate all of these factors into comparable indicator elements , each element's value is based on the release data, adjusted by weights reflecting the chemical's toxicity relative to other chemicals, the potential exposure caused by the emission, and the size of the potential exposed population. There are different equations for the human health and the ecological indicators, because each has different types of data available and different requirements for comparing the effect of releases of TRI chemicals. Both human and ecological indicator elements incorporate estimates of the uncertainties associated with component weights. By using toxicity, exposure potential, and population size adjustments to the emission, the changes in the indicators over time should be more closely related to changes in risk than changes in emission quantities alone.

The toxicity and exposure factors that are used to adjust the releases are referred to as weights. Briefly, the weights used to construct the TRI Environmental Indicators are derived by classifying a release in terms of ranges of toxicity, exposure, and population exposed, and assigning a weight value to each range. The weight assigned to each range increases proportionally as toxicity or exposure increase. The methodology for deriving weights is discussed in more detail below. It must be reiterated that while the resulting indicators are intended to relate to risk by considering toxicity, exposure and population factors, the indicators do not provide actual risk estimates.



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Toxicity Weights -- Human

For both carcinogenic and noncarcinogenic chronic effects, the proposed methodology for developing human health toxicity weights is based on scoring systems that include both qualitative and quantitative elements. There is uncertainty inherent in determining the potency of chemicals in causing human health effects, thus any quantitative potency data must be considered in the context of a qualitative classification of the uncertainty associated with that data. Therefore, the toxicity of each chemical is classified both quantitatively using potency data and qualitatively using weight-of-evidence (WOE). Both kinds of data are considered when deriving the score, and so both kinds of data must be generated for the TRI chemicals.

For human health, a number of quantitative measures of potency can be used for toxicity weighting. Commonly used quantitative measures include the $q_1^*$, which describes cancer potency; reference doses (RfDs) for non-carcinogens; and reportable quantities (RQs). The $q_1^*$s, and RfDs are toxicity measures that have been developed for EPA risk evaluation purposes. RQs have been developed using similar toxicity data reviews to mandate reporting of releases to EPA at various release volumes. One or more of these values are available for 247 TRI chemicals. There are some TRI chemicals for which there are currently no formal EPA toxicity evaluations; for these chemicals, potential toxicity will be evaluated based on toxicity data available from other data sources, as well as quantitative structure activity relationship methods, to supplement the formal available EPA toxicity values. For certain chemicals of extraordinary interest, special resources may have to be made available to perform an adequate toxicity evaluation. Chemicals for which little if any toxicity data exist, and thus no evaluation of toxicity is possible, will be excluded from the indicator calculation.

The second element of the human health toxicity weighting is the qualitative weight-of-evidence (WOE) classification schemes. There is an exception to this method, however. For chemicals with RfDs, WOE is considered in the development of an RfD; thus, consideration of WOE is already imbedded in the RfD value. Therefore, WOE is not used in this methodology for assigning toxicity weights for chemicals with RfDs. WOE information must be generated for carcinogens and for noncarcinogens without RfDs. The WOE schemes proposed in this report have been adopted from several sources. For cancer, the EPA Cancer Risk Assessment Guidelines[2] and the TSCA Chemical Scoring System[3]

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[2]U.S. Environmental Protection Agency (EPA). 1986a. Guidelines for Carcinogen Risk Assessment. 51 Federal Register 33992 (September 24, 1986), currently being revised.

[3]O'Bryan, T.R. and R.H. Ross. 1988. Chemical Scoring System for Hazard and Exposure Identification. Journal of Toxicology and Environmental Health, 1:119-134.

WOE schemes are used. Non-carcinogenic WOE guidelines from the TSCA Chemical Scoring System and from various EPA noncancer risk assessment guidelines are proposed for use for non-carcinogens without RfDs.

Using the quantitative toxicity data and qualitative weight of evidence information, chemicals are assigned to toxicity ranges and WOE categories. A matrix, with WOE categories on one axis and toxicity ranges on the other, are used to assign weights to each chemical. Separate matrices for carcinogens and noncarcinogens are used for human health toxicity. Proportional weights -- reflecting the magnitude of differences in toxicity between chemicals -- are assigned to the matrix cells. Weights increase by an order of magnitude for each order of magnitude increase in toxicity and for each increase in WOE category. For a chemical that causes multiple toxic effects, the TRI indicator will weight a chemical based on the endpoint associated with the lowest dose at which an effect occurs, but will not apply additional weights for severity relative to other health effects or for the number of effects caused.

**Toxicity Weights -- Ecological**

For ecological effects, the Indicator will focus on aquatic life impacts. Very little data are available for most chemicals on effects to terrestrial or avian species, and the human health indicator will provide some predictor of these. For aquatic effects, WOE qualifications of potency data are not used because direct quantitative evidence of toxicity is available in the form of ambient water quality criteria (AWQC), $LC_{50}$s (lethal concentration, 50 percent), no observable adverse effect levels (NOAELs), and aquatic RQs. Direct measures of bioaccumulation potential may be available in the form of laboratory-derived bioconcentration factors (BCFs) or bioaccumulation factors (BAFs). Where laboratory data are unavailable, one of two indicators of bioaccumulation potential can be used: either a measure of the potential for organic chemicals to partition between organic material and water, or the water solubility of the chemical.

For aquatic effects, two matrices will be used to develop separate weights for toxicity and bioaccumulation. Weights from each matrix are then multiplied for a final weight. Both matrices assign weights that increase by increments of an order of magnitude as toxicity and bioaccumulation potential increase.

**Exposure Weights -- Human**

For human exposure weighting, as with toxicity weighting, both quantitative and qualitative (uncertainty) elements are considered when weighting exposure potential. Three steps are involved in deriving the human exposure weight. The first step is to categorize some measure of exposure potential into numerical ranges. The second step is to categorize the levels of uncertainty associated with the measures of exposure potential. The final step uses a matrix, with numerical exposure potential ranges arrayed along one axis and



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uncertainty categories arrayed along the other, to assign increasing weights to higher-certainty/higher exposure potential releases.

For the first step of this process, quantitative measures of exposure potential must be estimated. To do so, several existing scoring systems take the approach of ordinally ranking the volume of each release by the some physical measure of the chemical's ability to move through the environmental medium into which it is released. However, because the exposure potential rankings would have different physical meanings for different pathways, comparisons among releases to different media would be difficult, and weighted releases from different pathways could not be added to obtain a single indicator value.

In this methodology, comparisons across media can be made because a common quantitative exposure measure for each medium is derived: an estimate of "surrogate dose" -- a measure related to the amount of chemical contacted by an individual per kg body weight per day. Although limited facility-specific data and the use of generic models (described below) prevent the calculation of an actual dose, the surrogate dose measure developed from the available data and from generic modeling is designed to be, in concept, comparable for all media.

To estimate the magnitude of exposure potential from TRI releases, the methodology uses generic environmental fate and transport models. A separate exposure evaluation is conducted for each release pathway (e.g., air, land, surface water). The exposure evaluations combine data on media-specific emission volumes, physicochemical properties, and where available, site characteristics with generic exposure models to determine an estimate of the magnitude of the ambient concentration of contaminant in the medium into which the chemical is released. (Again, the use of submitter-estimated TRI emission data and generic models with many default assumptions make this only a surrogate related to actual concentration). For the human health indicator, the ambient media concentrations are then combined with standard human exposure assumptions to estimate the magnitude of the surrogate dose.

It must be emphasized that while this methodology uses the EPA exposure assessment paradigm to evaluate exposure potential, the results should not be construed as an actual absolute numerical estimate of dose resulting from TRI releases. Instead, the purpose is to obtain an order of magnitude estimate of surrogate dose resulting from release of TRI chemicals *relative to the surrogate dose resulting from other releases included in the indicator*, so that these releases can be weighted appropriately in the indicator.

The modeling approach proposed by this methodology to obtain surrogate ambient concentrations and surrogate dose measures for each pathway is summarized below.

- Stack and Fugitive Air Emissions: The Gaussian dispersion algorithm from the Industrial Source Complex Long Term (ISCLT) model, with assumed stack height, Stability Array (STAR) weather data, and specified distances



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from the source is used to estimate the surrogate ambient concentrations of contaminants. For human exposure, the surrogate dose measure is estimated by combining population-weighted average air concentration with standard assumptions for inhalation rate and body weight.

- Direct Surface Water Releases: Stream flow data from the GAGE database is combined with release data and chemical half-lives to derive surrogate concentrations of chemicals in surface water. For human exposure, the concentration is combined with data on populations served by drinking water utilities with downstream intakes, bioconcentration factors, standard water ingestion rates, fish ingestion rates, and body weight assumptions to derive the surrogate dose.

- On-Site Land Releases: Volatilization and groundwater pathways were considered in deriving the indices. Volatilization release data are reported by the facilities with other air release data and are thus modeled with other fugitive air releases from the facility. Groundwater contamination is modeled only for disposal of TRI chemicals to onsite nonhazardous solid waste management units. (Chemicals contained in solid waste streams classified as hazardous are subject to additional disposal provisions which are assumed to significantly limit potential for groundwater release and human exposure). Leachate from landfills is modeled as a function of estimated concentration of contaminant in the landfill, the soil/water partition coefficient, and the bulk density of landfill material. The magnitude of dilution and attenuation of contaminants as they move toward drinking water wells are estimated according to existing EPA dilution and attenuation factors (DAFs). The surrogate dose measure is estimated for the population of well-water drinkers within a specified distance of the landfill site.

- Transfers to POTWs: The fate of chemicals entering POTWs is determined according to existing estimates of POTW removal efficiencies and within-POTW partitioning rates (i.e., the amount of contaminant that biodegrades, volatilizes, or is adsorbed to sewage sludge). The exposure to chemicals that are not removed by the POTW are modeled according to the methodology for direct surface water releases, while volatilized chemicals are modeled as area-source air releases.

- Other Off-Site Transfers: For off-site transfers, methodologies for modeling exposure are available for two disposal technologies: waste incineration and landfilling. Air releases from incineration are modeled in the same manner as other air releases, using removal efficiencies for nonhazardous waste incinerators. For landfills, groundwater exposures are modeled in the same manner as on-site disposal facilities. Unlike volatilization emissions from onsite facilities, volatilization emissions from off-site facilities are not



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reported, and must be estimated, then modeled for exposure potential. Once estimated, volatile emissions are then modeled in the same way as other air releases.

Investigations are continuing to examine methods for assessing underground injection, both on- and off-site, as well as other treatment methods used for off-site transfers. For the initial calculations of the TRI Environmental Indicators, these pathways will likely be considered as contributing negligible amounts to the exposure weight.

For the second step of the exposure weighting process, uncertainty categories are created by considering the relative uncertainties associated with modeling different exposure pathways, each of which will have a different level of modeling precision and dependability of site-specific data associated with it. This method uses three qualitative categories of increasing uncertainty to weight exposure estimates. The more uncertainty associated with an estimate, the less weight given the exposure estimate, with an order of magnitude difference between the categories with the highest and lowest estimates. (The middle uncertainty category is given a weight twice that of the category with the most uncertainty.)

**Exposure Weights -- Ecological**

For aquatic life exposure to TRI chemicals, a weight is assigned to each one of several categories of exposure, with order of magnitude ranges of ambient water concentrations of the chemical resulting from a release used to define potential exposure. The weights assigned to the ranges increase by an order of magnitude with each increasing range of contaminant concentrations.

Aquatic exposure weights for categories of increasing estimated water concentration do not need to reflect exposure relative uncertainty, since all estimates are derived using the same methodology. The weights simply increase by an order of magnitude for each category.

**Population Size Weights**

This methodology proposes several rules for the use of population size data in the exposure evaluation. First, a minimum population value is assumed to all releases to avoid undervaluing sparsely distributed or rural populations. Second, both qualitative data (on the uncertainty of the population size estimate) and quantitative data are used when evaluating the size of the population potentially exposed to TRI releases.

To reflect the uncertainty associated with the size of exposed human populations, population sizes are assigned to one of three qualitative categories of uncertainty, and are reduced by an order of magnitude for each level of uncertainty. All population sizes are rounded up to the nearest 1,000 persons, thus creating a minimum exposed population.



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Because of the major difficulties in estimating sizes of the populations of ecological receptors, the TRI Ecological Indicator does not include a population weight. In effect, this approach assumes that all aquatic emissions occur to equally vulnerable locations.

## COMPUTATION OF THE INDICATORS

Each indicator's value is generated by a computer algorithm which links input files of releases and other input data required to mathematical models of media-specific pathway releases, which are then linked to toxicity and exposure weighting factors to produce indicator elements. The program generates up to 500,000 such elements , which are summed to produce the values for each of the four indicators.

The elements can also be combined and evaluated in other ways than annual comparisons. The detailed calculations used to create elements allow computation of subindicators for individual chemicals, geographic regions, industry sectors, facilities, or exposure pathways. These subindicators, like the overall indicator, cannot be compared to some absolute level of concern, but could help identify the relative contribution to various components to the overall estimate of emission impacts.

## ISSUES FOR FUTURE CONSIDERATION

There are two general types of issues: specific methodological questions for the indicators developed to date, and development of additional indicators. The methodological questions associated with the indicators developed to date that still need to be resolved include the following:

- How to address additions/deletions to the TRI chemical list, and whether to create new indicators when significant changes are made;
- How to include deposition of TRI chemicals into underground injection wells in the indicators;
- For noncarcinogenic chemicals without RfDs, what specific WOE systems should be used for neurotoxicity, reproductive toxicity, and other chronic toxicity endpoints;
- For offsite transfers, how to better match TRI transfers to particular treatment practices (e.g., which TRI chemicals are sent to hazardous or nonhazardous waste management facilities; use of specific treatment practices at POTWs; and how to estimate the potential impact of non-landfill, non-incineration treatment types); and
- Using initial results of indicator computations, examine the impact of various exposure weights and their WOE modifiers.

The possible development of indicators for acute human health effects and acute aquatic effects depends on improved toxicity and other data. In addition, EPA considered expanding the TRI Environmental Indicators to reflect indirect health and environmental risks from TRI chemicals, such as global climate change, acid deposition, stratospheric ozone depletion, tropospheric ozone formation, and particulate deposition. While many of these impacts have health-related effects, the complexity and uncertainty in modeling them may make it impossible to incorporate them into the present set of indicators.

## CONCLUSION

As an indication of improvements in environmental quality over time, the Human Health and Ecological indicators provide the EPA with a valuable tool to measure general trends related to impacts of TRI chemicals. They do not capture all environmental releases of concern, and thus changes in these indicators over time cannot be used to evaluate changes in other sources of environmental pollution. These indicators do, however, generally relate changes in releases to relative changes in chronic human health and ecological risks from a large number of toxic chemicals of concern to the Agency. Importantly, the indicators also provide an ability to analyze the relative contribution of source categories to important changes.

# I. INTRODUCTION

In 1989, EPA Administrator William Reilly outlined the goals and processes for establishing a strategic planning and accountability process at the Agency. Underlying this approach is the Agency's desire to set priorities and shift resources to areas with the greatest opportunity to achieve health risk and environmental risk reductions. As part of this initiative, the Administrator set forth a plan to develop indicators of environmental progress in achieving the Agency's goals. Tracking this progress will allow the Agency to measure its successes in implementing environmental protection and pollution prevention programs, and to formulate strategic plans for improving the course of future environmental progress.

Within the Office of Pollution Prevention and Toxics (OPPT), environmental indicators were identified as a component of the Toxic Substances Program Strategy 1992 - 1995. The strategy described an indicator that would reflect environmental exposures as the Dow Jones Average reflects the behavior of the New York Stock Exchange. The strategy envisioned that the indicator will provide an estimate of emissions reductions across media, including reductions that are voluntary on the part of industry and those that are a result of government actions.

In general terms, such an indicator will allow EPA to track changes in human health and environmental impacts from emissions over time. As such, the Agency will need to take advantage of existing data sources that reflect multimedia trends in environmental contaminant releases. One such database, the Toxic Release Inventory (TRI), is the OPPT's most relevant source of data for developing an annual indicator of environmental progress. TRI is mandated by the Superfund Amendment Reauthorization Act (SARA) Title III Section 313 and requires that U.S. manufacturing facilities file annual reports documenting multimedia environmental releases and off-site transfers for over 300 chemicals which are of concern to the Agency. Therefore, any indicator built from TRI data will be primarily an indicator for the manufacturing sector. However, despite the fact that the TRI database does not capture all chemicals, industrial sectors, or releases of concern to both OPPT and the Agency as a whole, the database is the Agency's single best source of consistently reported release data. Moreover, SARA Section 313 explicitly provides for the expansion of TRI to cover additional chemicals and industries, and a major effort is currently underway to add key chemicals and industries to TRI. Furthermore, other program offices in the Agency are in the process of developing indicators that will complement the TRI indicator.

The TRI "indicator" may eventually consist of a set of four indicators. The focus of this report is the development of indicators of chronic human health impacts and aquatic life impacts. The development of corresponding acute effects indicators is not feasible now, since the data to support such indicators are not available. To appropriately evaluate potential acute effects, one would need to know the distribution of releases over time (peak release data), and these data are not currently reported to TRI. However, possible changes



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in reporting requirements may allow for the development of separate acute indicators for human and ecological effects.

The ultimate goal of the indicator effort is to devise a measure that reflects the impacts of chemical releases and transfers, which can be used to assess progress in reducing these impacts over time. The indicator methodology should be comprehensible, replicable, and easily adaptable to a computer program. The methodology should also be sufficiently flexible to facilitate separate analyses of indicator components, including specific media, industrial sectors, chemicals, and geographic areas. The methodology should also have provisions that either provide for uncertainty or provide alternatives when data are unavailable. The method should be sufficiently flexible to permit updates as new chemicals/industries are added to TRI. Finally, all assumptions on which the indicators are based should be easily identifiable and understood.

This report explains how the proposed TRI Environmental Indicators are constructed, and includes discussions of the conceptual methodology, data sources, and computational approach. The proposed indicators are based on risk-related scores, and the report discusses the similarities and distinctions between the risk-based approach of the indicators and conventional risk assessments.

In developing the proposed indicators, many approaches to assessing and ranking the potential impact of chemicals were reviewed. Numerous techniques to score the relative significance of TRI chemicals and facilities have been and continue to be developed. One objective of this report is to explain the indicators to a variety of agencies and groups that may wish to use or adapt the indicators or the methodologies to their own needs. A related objective is to describe the benefits of the proposed approach to the indicators in terms of flexibility, power as an analytical tool, and usefulness as a policy tool.

## II. GENERAL DESCRIPTION OF THE TRI ENVIRONMENTAL INDICATORS

The objective of the indicator methodology presented in this report is to construct a unitless value related to the overall impacts of releases and transfers of all included TRI chemicals by all facilities to each environmental medium at a given point in time. The indicators are planned to be calculated each year based on the most current TRI data, and compared to previous years' indicator values. One of the early years of TRI reporting, e.g. 1989, would be selected as a "base year" and later years' indicator values compared to it. For the base year, the unitless score would be normalized to a round number such as 10,000; subsequent years' data would be normalized by the same factor to provide a relative comparison. This will allow assessment of the changes in estimated impacts of TRI releases and transfers from year to year.



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Four components are generally used to compute each indicator (e.g. for human health chronic impacts). These are:

- the quantity of a chemical released or transferred,
- a toxicity adjustment,
- an adjustment reflecting the size of the potentially exposed population, and
- an exposure potential adjustment.

Separate assessments are made for each unique combination of a chemical, facility, and release medium. For each of these releases or transfers, one develops an indicator "element": a unitless value proportional to the potential impact of each specific release or transfer. The value for each TRI indicator is simply the sum of all the indicator elements.

It must be emphasized that the TRI Environmental Indicator methodology is not intended to be a quantitative risk assessment and does not calculate risk estimates. The proposed methodology utilizes some of the tools often applied in quantitative assessments, but in a relative way. The TRI Environmental Indicators are by their nature only intended to reflect the direction and the general magnitude of the change in releases over time, scaled by factors (toxicity, exposure potential, receptor population size) that relate to potential risk. As such, an indicator value has only relative rather than absolute meaning; it can only be used in comparisons to other values at different points in time, or in identifying the relative size of contributing factors.

Human Health Chronic Indicator

Each element of the Human Health Chronic Indicator (each of which is facility-chemical-medium-specific) consists of three components: toxicity, exposure (which includes release size), and the size of the exposed population. Components are multiplied to calculate the element. It must be reiterated that an element value is not an absolutely meaningful measure of risk associated with the facility. These values are useful as an approximate measure that is comparable to approximate measures for other facilities calculated using the same methods, to identify relative significance.

The current proposal is focused on general populations: individuals, particularly highly exposed individuals, are not the focus of the indicator. Additional indicators based upon highly exposed or sensitive subpopulations may be developed in the future.

Ecological Chronic Indicator

For the Ecological (aquatic life) Chronic Indicator, the elements are developed by combining aquatic toxicity and exposure components for each facility, each chemical, and each medium. As with the Human Health Chronic Indicator, each component contributes multiplicatively to the overall magnitude of the element value. For the Ecological Chronic Indicator, the population component is not utilized, since the size of the exposed population



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is typically not known, and because of the difficulty in relating impacts to ecological systems with many exposed populations of organisms.

There are several factors that must be considered in constructing the indicators: these include selecting chemicals for inclusion, designing a mechanism for adjusting emissions to reflect exposure and toxicity, and developing algorithms for calculating these adjustments. The following sections describe the elements of the proposed TRI indicators. A conceptual flow chart of the proposed TRI Environmental Indicator methodology is presented in Figure 1.

## III. SELECTION OF CHEMICALS AND FACILITIES TO INCLUDE IN THE INDICATORS

### Selection of Chemicals

In order to be as inclusive as possible and still maintain computational tractability, a large subset of TRI chemicals should be included in the indicators. However, several factors must be considered when determining whether to include a chemical in the indicators calculation. The number of chemicals included in the indicators could be limited by the availability of data characterizing the chemical or the magnitude of emissions.

The TRI Environmental Indicator Work Group initially identified the following list of criteria for selecting chemicals to exclude from the TRI indicators:

- Criterion 1: Exclude chemicals with no reporting or zero reporting. For 1989 TRI data, these criteria alone would exclude 73 chemicals and over 2000 facilities from consideration, leaving 244 chemicals and over 20,000 facilities included in the TRI indicators analysis. The chemicals excluded by these criteria are listed in Table 1. These criteria would allow the Agency to concentrate resources (such as the research on toxicity and environmental fate data) on those chemicals that could actually cause a potential impact. One problem with this approach is that the potential future increase of emissions of these chemicals could contribute to health and environmental impacts. However, reporting of increased emissions of chemicals could result in their addition to the indicators. This issue is covered in a later discussion of the normalization of the indicators. Because it is possible that some facilities may incorrectly report zero releases, this criterion could be limited to excluding chemicals with no reporting. In this case, the criterion would exclude 53 chemicals from the indicators analysis, but no facilities, since if chemicals have no reports, presumably no facility in the database would have only these chemicals on its form R.



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# Figure 1

**Methodology for Calculating Human Health TRI Indicator**

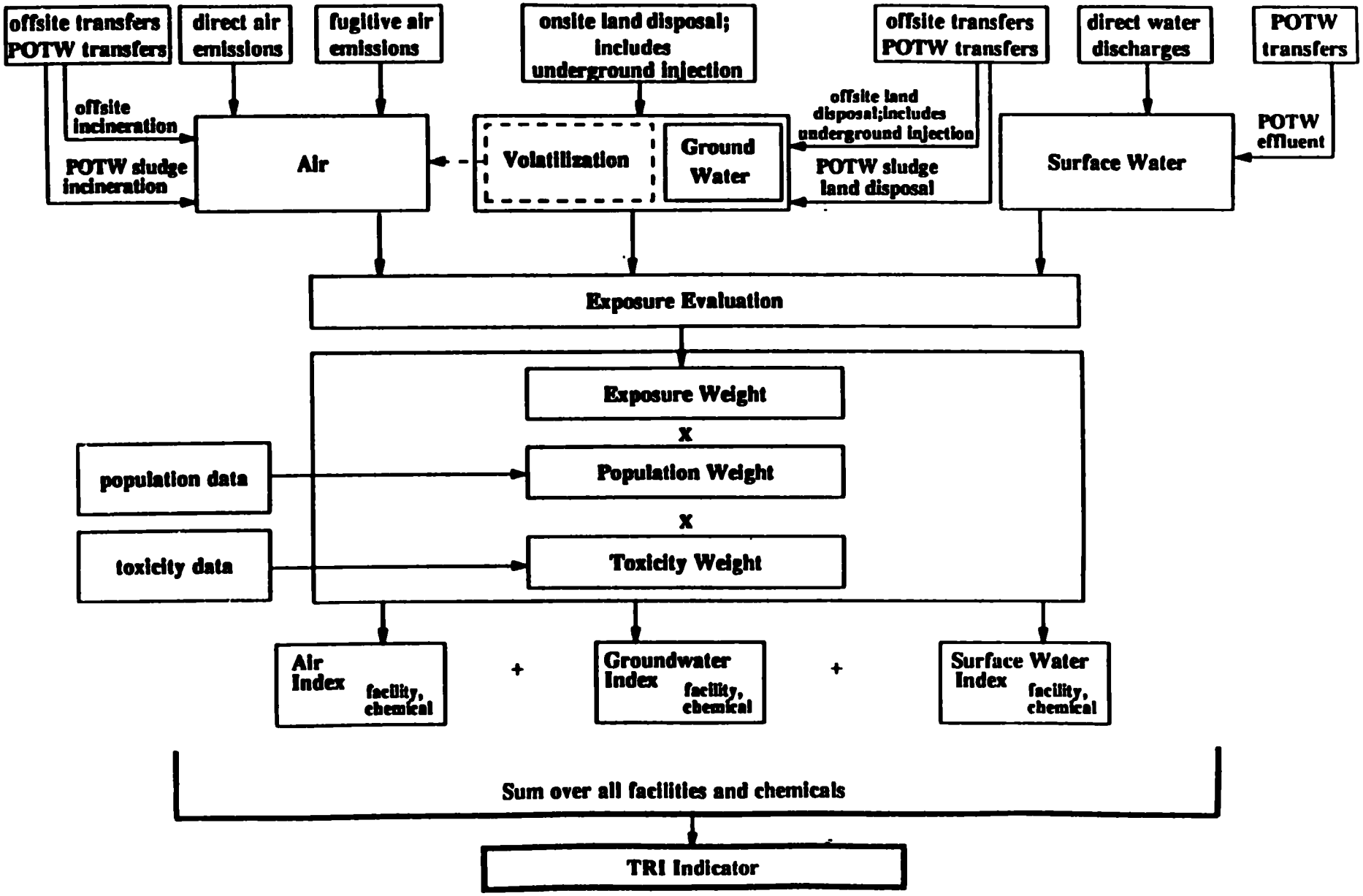

Table 1
Chemicals With No Reports or No Reported Releases (73 Total)
Shaded Chemicals Were Reported but With No Releases (20 Total)
Total number of chemicals(73) and facilities (>2000)
1989 Toxics Release Inventory Data

| CAS | Chemical |
|---|---|
| 51752 | NITROGEN MUSTARD |
| 53963 | ACETYLAMINOFLUORENE,2 |
| 55185 | NITROSODIETHYLAMINE,N |
| 57125 | CYANIDE |
| 57578 | PROPIOLACTONE,BETA |
| 59892 | NITROSOMORPHOLINE,N |
| *60093* | *AMINOAZOBENZENE, 4* |
| 60117 | DIMETHYLAMINOAZOBENZENE,4 |
| *60355* | *ACETAMIDE* |
| *62759* | *NITROSODIMETHYLAMINE,N* |
| 68768 | TRIAZIQUONE |
| 75274 | DICHLOROBROMOMETHANE |
| 79447 | DIMETHYLCARBAMYL CHLORIDE |
| *81889* | *C.I. FOOD RED 15* |
| 82280 | 1-AMINO 2-METHYL-ANTHRAQUINONE |
| 91598 | NAPHTHYLAMINE, BETA |
| *92671* | *AMINODIPHENYL,4* |
| 92875 | BENZIDINE |
| 92933 | NITROBIPHENYL,4 |
| *95954* | *TRICHLOROPHENOL, 2,4,5* |
| 96128 | DIBROMOCHLOROPROPANE (DBCB) |
| *97563* | *C.I. SOLVENT YELLOW 3* |
| *99592* | *NITROOANISIDINE, 5* |
| 100754 | NITROSOPIPERIDINE,N |
| *101804* | *DIAMINODIPHENYLETHER, 4,4* |
| *104949* | *ANISIDINE,P* |
| *107302* | *CHLOROMETHYL METHYL ETHER* |
| *114261* | *PROPOXUR* |
| 115532 | DICOFOL |
| 117793 | AMINOANTHRAQUINONE,2 |
| *119904* | *DIMETHOXYBENZIDINE, 3,3* |
| 119937 | DIMETHYLBENZIDINE, 3,3 |
| 122667 | DIPHENYLHYDRAZINE, 1,2 |
| 126727 | TRIS(2,3DIBROMOPROPYL)PHOSPHATE |
| 128665 | C.I. VAT YELLOW 4 |
| 134292 | ANISIDINE HYDROCHLORIDE,O |
| 135206 | CUPFERRON |
| 139651 | THIODIANILINE,4,4 |
| 309002 | ALDRIN |
| 334883 | DIAZOMETHANE |
| 492808 | AURAMINE |

Table 1
Chemicals With No Reports or No Reported Releases (73 Total)
Shaded Chemicals Were Reported but With No Releases (20 Total)
Total number of chemicals(73) and facilities (>2000)
1989 Toxics Release Inventory Data

| CAS | Chemical |
|---|---|
| 505602 | MUSTARD GAS |
| 510156 | CHLOROBENZILATE |
| 532274 | CHLOROACETOPHENONE |
| *542881* | *BIS(CHLOROMETHYL)ETHER* |
| *615054* | *DIAMINOANISOLE,2,4* |
| 621647 | NITROSODInPROPYLAMINE,N |
| 636215 | TOLUIDINE HYDROCHLORIDE |
| 680319 | HEXAMETHYLPHOSPHORAMIDE |
| 684935 | NITROSONMETHYLUREA,N |
| 759739 | NITROSONETHYLUREA,N |
| *842079* | *C.I. SOLVENT YELLOW 14* |
| 924163 | NITROSODInBUTYLAMINE,N |
| *989388* | *C.I. BASIC RED 1* |
| *1120714* | *PROPANE SULTONE* |
| 1335871 | HEXACHLORONAPHTHALENE |
| 1464535 | DIEPOXYBUTANE |
| 1836755 | NITROFEN |
| 1937377 | C.I. DIRECT BLACK 38 |
| 2234131 | OCTACHLORONAPHTAHLENE |
| 2303164 | DIALLATE |
| 2602462 | C.I. DIRECT BLUE 6 |
| *2832408* | *C.I. DISPERSE YELLOW 3* |
| 3118976 | C.I. SOLVENT ORANGE 7 |
| 3761533 | C.I. FOOD RED 5 |
| 4549400 | NITROSOMETHYLVINYLAMINE,N |
| 4680788 | C.I. ACID GREEN 3 |
| 7440280 | THALLIUM |
| 8001352 | TOXAPHENE |
| 16071866 | C.I. DIRECT BROWN 95 |
| 16543558 | NITROSONORNICOTINE,N |
| 20816120 | OSMIUM TETROXIDE |
| *39156417* | *DIAMINOANISOLE SULFATE, 2,4* |



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- Criterion 2: Exclude chemicals with relatively low reporting (between 1 and 1,000 lbs to each medium: air, water, land, off-site transfers, transfers to POTWs). Excluding these chemicals would allow us to focus the indicators on chemicals causing the greatest impacts. The danger of this criterion is the possibility of excluding a high-toxicity but low-volume release that may contribute substantially to health and environmental impacts. Another problem with this approach is the potential future increase of emissions of these chemicals that could contribute to risk. This criterion would exclude 12 chemicals but fewer than 5 facilities from consideration. Those chemicals that would be excluded by this criterion are found in Table 2. Some Work Group members suggested increasing the cutoff for off-site transfers to 25,000 lbs, since such transfers may undergo treatment before release to the environment. Increasing the exclusion criterion for offsite transfers to less than 25,000 lbs. would exclude 19 chemicals and about 10 facilities.

- Criterion 3: Exclude chemicals with relatively low reporting (between 1 and 1,000 lb to all media combined: air, water, land, off-site transfers, transfers to POTWs). Similar to the previous criterion, this would allow us to concentrate on chemicals causing the greatest impacts, but may exclude high toxicity, low volume releases and encourage future emission increases that would contribute to environmental impacts. This criteria would exclude 7 chemicals but fewer than 5 facilities from consideration. Those chemicals excluded by this criterion are found in Table 3.

- Criterion 4: Exclude chemicals having no toxicity data. As discussed briefly above, the TRI Environmental Indicators will require incorporation of data on the relative toxicity of chemicals. Chemicals must be scored based on available toxicity data. If there is insufficient information upon which to evaluate the toxicity of a chemical, the chemical would be excluded from the indicators. It should be emphasized that exclusion from the indicators would be a last resort, used only after all available mechanisms for closing data gaps (including structure activity relationship methods and best professional judgment) are exhausted. While this criterion presents a danger of excluding risky but poorly studied chemicals, the risk-related nature of the indicators does not allow for inclusion of these chemicals. Table 4 presents the TRI chemicals for which formal EPA toxicity data are not available in the Integrated Risk Information System (IRIS) or in the Health Effects Assessment Summary Tables, and for which specific health-based (chronic, carcinogenic) Reportable Quantities have not been developed under CERCLA. As shown in this table, there are 70 chemicals that have no readily available toxicity data. Thirty-three of these 70 have zero or no reported releases. Excluding these 70 chemicals would exclude about 250 facilities. This table will be circulated among other OPPT divisions and other Agency offices (such as the Pesticides office) to solicit additional available toxicity



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Table 2
Chemicals With TRI Releases Less Than 1,000 Pounds in Each Media
(Air, Water, Land, Off–site Transfers, Transfers to POTWs)
Total Number of Chemicals is 12 and Number of Facilities is Less than 5
1989 Toxics Release Inventory Data

| CAS | CHEMICAL |
|---|---|
| 55210 | BENZAMIDE |
| 60344 | METHYL HYDRAZINE |
| 72435 | METHOXYCHLOR |
| 75558 | PROPYLENEIMINE |
| 88891 | PICRIC ACID (2,4,6TRINITROPHENOL) |
| 94597 | SAFROLE |
| 96093 | STYRENE OXIDE |
| 134327 | NAPHTHYLAMINE, ALPHA |
| 156105 | NITROSODIPHENYLAMINE, P |
| 593602 | VINYL BROMIDE |
| 10034932 | HYDRAZINE SULFATE |
| 12122677 | ZINEB |



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**Table 3**
**Chemicals With TRI Releases Between 1 and 1,000 Pounds Across All Media (Air, Water, Land, Off–site Transfers, Transfers to POTWs)**
**Total Number of Chemicals is 7 and Number of Facilities is Less Than 5**
**1989 Toxics Release Inventory Data**

| CAS | CHEMICAL |
|---|---|
| 60344 | METHYL HYDRAZINE |
| 75558 | PROPYLENEIMINE |
| 88891 | PICRIC ACID (2,4,6TRINITROPHENOL) |
| 94597 | SAFROLE |
| 134327 | NAPHTHYLAMINE, ALPHA |
| 156105 | NITROSODIPHENYLAMINE, P |
| 10034932 | HYDRAZINE SULFATE |



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Table 4

C[illegible]cals With No Widely Available EPA Toxicity Data (IRIS, HEAST, human health RQs)

To[illegible]umber of chemicals (70) and facilities (about 250)

Shaded chemicals have zero or no reported releases (31)

| CAS | Chemical | Comment re: potential data |
|---|---|---|
| 20075 | COBALT COMPOUNDS | |
| 55210 | BENZAMIDE | |
| 55630 | NITROGLYCERIN | teratogen |
| 59892 | NITROSOMORPHOLINE,N | |
| 60093 | AMINOAZOBENZENE, 4 | |
| 60355 | ACETAMIDE | NTP carcinogen |
| 64675 | DIETHYL SULFATE | |
| 67630 | ISOPROPYL ALCOHOL FOR STRONG ACID PURPOSES | |
| 68768 | TRIAZIQUONE | |
| 74851 | ETHYLENE | |
| 78842 | ISOBUTYRALDEHYDE | |
| 81889 | C.I. FOOD RED 15 | |
| 82280 | 1-AMINO 2-METHYL-ANTHRAQUINONE | |
| 87627 | XYLIDINE,2,6 | NTP carcinogen |
| 88891 | PICRIC ACID (2,4,6TRINITROPHENOL) | |
| 90040 | ANISIDINE,O | |
| 90948 | MICHLERS KETONE | |
| 91087 | TOLUENE2,6DIISOCYANATE | potential carcinogen |
| 92671 | AMINODIPHENYL,4 | |
| 92933 | NITROBIPHENYL,4 | |
| 94360 | BENZOYL PEROXIDE | |
| 95636 | TRIMETHYLBENZENE, 1,2,4 | |
| 96093 | STYRENE OXIDE | potential carcinogen |
| 97563 | C.I. SOLVENT YELLOW 3 | |
| 99592 | NITROOANISIDINE, 5 | |
| 101688 | METHYLENEBIS(PHENYLISOCYANATE) | |
| 101779 | METHYLENEDIANILINE,4,4 | potential carcinogen |
| 101804 | DIAMINODIPHENYLETHER, 4,4 | |
| 104949 | ANISIDINE,P | |
| 111422 | DIETHANOLAMINE | |
| 115071 | PROPYLENE (PROPENE) | |
| 117793 | AMINOANTHRAQUINONE,2 | |
| 120718 | CRESIDINE,P | |
| 120809 | CATECHOL (1,2 DIHYDROXYBENZENE) | potential carcinogen |
| 123386 | PROPIONALDEHYDE | |
| 123728 | BUTYRALDEHYDE | |

Table 4

Chemicals With No Widely Available EPA Toxicity Data (IRIS, HEAST, human health RQs)

Total number of chemicals (70) and facilities (about 250)

Shaded chemicals have zero or no reported releases (31)

| CAS | Chemical | Comment re: potential data |
|---|---|---|
| 128665 | C.I. VAT YELLOW 4 | |
| 132649 | DIBENZOFURAN | |
| 134292 | ANISIDINE HYDROCHLORIDE,O | |
| 135206 | CUPFERRON | CAA Section 111 |
| 139139 | NITRILOTRIACETIC ACID | |
| 139651 | THIODIANILINE,4,4 | |
| 141322 | BUTYL ACRYLATE | CAA – Section 111 and TSCA 8a |
| 156105 | NITROSODIPHENYLAMINE, P | |
| 156627 | CALCIUM CYANAMIDE | CAA – Section 111 and pesticide |
| 334883 | DIAZOMETHANE | |
| 463581 | CARBONYL SULFIDE | CAA – Section 112 |
| 541413 | ETHYL CHLOROFORMATE | |
| 569642 | C.I. BASIC GREEN 4 | |
| 615054 | DIAMINOANISOLE,2,4 | |
| 680319 | HEXAMETHYLPHOSPHORAMIDE | |
| 842079 | C.I. SOLVENT YELLOW 14 | |
| 989388 | C.I. BASIC RED 1 | |
| 1313275 | MOLYBDENUM TRIOXIDE | |
| 1314201 | THORIUM DIOXIDE | |
| 1335871 | HEXACHLORONAPHTHALENE | |
| 1836755 | NITROFEN | |
| 2234131 | OCTACHLORONAPHTAHLENE | |
| 2832408 | C.I. DISPERSE YELLOW 3 | |
| 3118976 | C.I. SOLVENT ORANGE 7 | |
| 3761533 | C.I. FOOD RED 5 | |
| 4680788 | C.I. ACID GREEN 3 | |
| 6484522 | AMMONIUM NITRATE | |
| 7440484 | COBALT | |
| 7664939 | SULFURIC ACID | |
| 7783202 | AMMONIUM SULFATE | |
| 10049044 | CHLORINE DIOXIDE | |
| 16543558 | NITROSONORNICOTINE,N | |
| 39156417 | DIAMINOANISOLE SULFATE, 2,4 | |



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data. For several of these chemicals (indicated in the comment column in Table 4), toxicity data are likely to be available within OPTS. Remaining data gaps could be filled with additional research and application of professional judgment. Again, chemicals would be excluded based on this criterion only after all means to fill data gaps had been exhausted. If new toxicity data became available, the chemical could later be added to the indicators (see Section VI for a discussion of normalizing the indicators with the addition of new chemicals).

- Criterion 5: Exclude chemicals with relatively low toxicity concerns. Excluding chemicals with low toxicity relative to other TRI chemicals allows us to focus on thoroughly evaluating those chemicals with the highest potential for contribution to the indicators. Criteria would be defined for "relatively low toxicity," based on specific toxicity threshold values. This criterion may exclude certain chemicals that have relatively low toxicity but have very high volume releases. Table 5 lists chemicals that would be excluded if low human health toxicity were defined as follows: (a) smallest reportable quantity equals 5,000 pounds; (b) oral and inhalation reference doses are greater than 0.1 mg/kg-day; or (c) oral and inhalation cancer potencies are less than 0.01 kg-day/mg. These criteria would exclude 37 chemicals and about 3000 facilities from consideration.

- Exclude chemicals meeting two or more of these criteria. A combination of the previous criteria would remove those chemicals with both relatively low toxicities and low releases, thus avoiding the loopholes discussed above. Possible combinations include: chemicals with low reporting to each media and low toxicity (Criterion 6); chemicals with low releases to all media combined and low toxicity (Criterion 7); and chemicals with no reports or zero releases and low toxicity (Criterion 8). This step would exclude those chemicals of minimal concern; these chemicals would be subject to addition in later years, if their reported releases increase above the established criteria. Based on 1989 TRI data, however, no chemicals would be eliminated using Criteria 6 and 7. Criterion 8 would exclude one chemical but no facilities from consideration.

- Possibly exclude "non-TSCA" chemicals. OPPT may wish to focus its indicators on those chemicals over which it has direct regulatory authority, e.g., those chemicals listed on the TSCA inventory (40 CFR §372.65). By doing so, the indicators could track OPPT program effectiveness; changes in TSCA chemical releases would not be masked by increases in releases of chemicals over which OPPT has no regulatory control. For example, there are a number of pesticides on the TRI roster (listed in Table 6), which may exclusively have uses that are not included on the TSCA inventory. This criterion would exclude few chemicals, since almost all chemicals in TRI are



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Table 5
Chemicals With Low Toxicity
Total number of chemicals(37) and facilities (about 3000)

| CAS | Chemical |
|---|---|
| 67561 | METHANOL |
| 67641 | ACETONE |
| 71363 | BUTYL ALCOHOL, N |
| 75003 | CHLOROETHANE (ETHYL CHLORIDE) |
| 75070 | ACETALDEHYDE |
| 75252 | BROMOFORM (TRIBROMOMETHANE) |
| 75274 | DICHLOROBROMOMETHANE |
| 75569 | PROPYLENE OXIDE |
| 78875 | DICHLOROPROPANE, 1,2 |
| 78922 | BUTYL ALCOHOL, SEC |
| 79061 | ACRYLAMIDE |
| 79107 | ACRYLIC ACID |
| 84662 | DIETHYL PHTHALATE |
| 85449 | PHTHALIC ANHYDRIDE |
| 85687 | BUTYL BENZYL PHTHALATE |
| 86306 | NITROSODIPHENYLAMINE,N |
| 90437 | PHENYLPHENOL, 2 |
| 98828 | CUMENE |
| 98873 | BENZAL CHLORIDE |
| 100425 | STYRENE |
| 103231 | BIS(2ETHYLHEXYL)ADIPATE |
| 106898 | EPICHLOROHYDRIN |
| 107211 | ETHYLENE GLYCOL |
| 108101 | METHYL ISOBUTYL KETONE |
| 108316 | MALEIC ANHYDRIDE |
| 108883 | TOLUENE |
| 108952 | PHENOL |
| 120127 | ANTHRACENE |
| 131113 | DIMETHYL PHTHALATE |
| 133062 | CAPTAN |
| 140885 | ETHYL ACRYLATE |
| 1582098 | TRIFLURALIN |
| 7440508 | COPPER |
| 7440666 | ZINC |
| 7647010 | HYDROCHLORIC ACID |
| 7664382 | PHOSPHORIC ACID |
| 7782505 | CHLORINE |

Note: This list includes only those chemicals that have EPA toxicity data.



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**Table 6**
**Pesticides Listed in TRI (that may have uses not covered under TSCA)**

| CAS | Chemical |
|---|---|
| 000052-68-6 | TRICHLOROFON |
| 000056-38-2 | PARATHION |
| 000057-74-9 | CHLORDANE |
| 000058-89-9 | LINDANE |
| 000062-73-7 | DICHLORVOS |
| 000063-25-2 | CARBARYL |
| 000072-43-5 | METHOXYCHLOR |
| 000076-44-8 | HEPTACHLOR |
| 000082-68-8 | QUINTOZENE |
| 000087-86-5 | PENTACHLOROPHENOL |
| 000088-06-2 | TRICHLOROPHENOL (2,4,6-) |
| 000094-75-7 | 2,4-D |
| 000095-95-4 | 2,4,5-TRICHLOROPHENOL |
| 000096-12-8 | DIBROMO-3-CHLOROPROPANE (1,2-) |
| 000106-93-4 | DIBROMOETHANE (1,2-) |
| 000114-26-1 | PROPOXUR |
| 000115-32-2 | DICOFOL |
| 000133-06-2 | CAPTAN |
| 000133-90-4 | CHLORAMBEN |
| 000309-00-2 | ALDRIN |
| 000510-15-6 | CHLOROBENZILATE |
| 000961-11-5 | TETRACHLORVINPHOS |
| 001582-09-8 | TRUFLURALIN |
| 001836-75-5 | NITROFEN |
| 001897-45-6 | CHLOROTHALONIL |
| 002164-17-2 | FLUOMETURON |
| 002303-16-4 | DIALLATE |
| 008001-35-2 | TOXAPHENE |
| 012122-67-7 | ZINEB |
| 012427-38-2 | MANEB |



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subject (at least theoretically) to TSCA authority. Exclusion of these chemicals could also diminish the usefulness of the indicators outside of OPPT if this criterion leads to the exclusion of a chemical of concern to another office.

Table 7 summarizes the number of chemicals and the number of facilities included and excluded by Criteria 1 through 8, discussed above. The Work Group also considered the idea of a selecting a random sample of the TRI chemicals for inclusion in the indicators. However, it was determined that a large percentage of the TRI roster (over 200 chemicals out of 317) would have to be selected in order to obtain an adequate representative sample with a sufficiently moderate coefficient of variation. Therefore, the Work Group concluded that randomly selecting chemicals would not be a fruitful exercise at this point. If, in the future, the TRI reporting system is expanded to contain a much larger number of chemicals, this option may be revisited.

In consideration of these criteria, this method proposes the exclusion of the following chemicals from the TRI indicators calculation:

- chemicals with either no reports, or only reports listing zero releases and transfers;
- chemicals with no available, EPA-reviewed toxicity data (but flag these); and
- possibly exclude chemicals with total releases to each medium below some threshold (e.g., 1000 pounds).

Note that chemicals of special interest to various offices in the Agency (such as chemicals undergoing regulatory activity) may inadvertently be excluded from the indicators based on one or more of these criteria. Once the final list of excluded chemicals is created, it can be examined to ensure that chemicals of special concern to the Agency are not excluded. In addition, other offices will be asked if there are chemicals that we have included that should in fact be excluded, such as pesticides that have not been nor will be reregistered for use in the U.S.

Inclusion of Facilities

Eliminating certain chemicals from the indicators will eliminate some facilities that release these chemicals from the indicators. There may be additional reasons to exclude certain facilities from the indicators. For example, the reliability of reporting from certain facilities may be questionable. There may also be concerns about the resource and computing requirements for including all facilities in the indicators. For these reasons, the Work Group considered options where a subset of facilities would be selected for inclusion in the indicators. Several statistical methods for selecting representative facilities were considered. Ultimately, the Work Group decided to include all facilities emitting the



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**Table 7**
**Proposed Criteria for Eliminating Chemicals**

| Criteria | Number of Chemicals Excluded | Number of Chemicals Remaining | Number of Facilities Excluded | Number of Facilities Remaining |
|---|---|---|---|---|
| 1 Chemicals with no or zero reporting of TRI releases | 73 | 244 | ~2200 | ~20,300 |
| 2 Chemicals with TRI releases less than 1,000 pounds in each media | 12 | 305 | <5 | ~22,500 |
| 3 Chemicals with TRI releases less than 1,000 pounds across all media | 7 | 247 | <5 | ~22,500 |
| 4 Chemicals with no EPA toxicity data | 70 | 243 | ~250 | ~22,250 |
| 5 Chemicals classified with low toxicity | 37 | 280 | ~3000 | ~19,500 |
| 6 Chemicals meeting Criteria 2 and 5 | 0 | 317 | 0 | ~22,500 |
| 7 Chemicals meeting Criteria 3 and 5 | 0 | 317 | 0 | ~22,500 |
| 8 Chemicals meeting Criteria 1 and 5 | 1 | 316 | 0 | ~22,500 |

chemicals included in the indicators. This approach avoids questions of representativeness of a selected subset of facilities. The Work Group also judged the inclusion of all facilities to be feasible within the resource constraints given the proposed approach described below.

## IV. METHODS FOR ADJUSTING EMISSIONS FOR TOXICITY AND EXPOSURE

To construct indicator elements that are related to risk, TRI emissions must be adjusted in a manner that relates to the risks associated with each media-specific release or transfer of each chemical. The risk potentially posed by a chemical emission depends on the inherent toxicity of the chemical, the environmental fate and transport of the chemical in the medium to which it is released, the degree of contact between the contaminated medium and the human or ecological receptors, and the size of exposed populations. Differences in toxicity among chemicals, as well as differences in environmental fate and in the size and characteristics of populations potentially exposed influence the relative contribution each emission makes to each indicator. Transfers to offsite locations such as sewage treatment plants (POTWs) require an additional estimate of the impact of treatment technology on the emissions.

In order to incorporate all of these factors into comparable indicator elements, each element's value is based on the release data, adjusted to reflect the chemical's toxicity relative to other chemicals, the potential exposure caused by the emission, and the size of the potential exposed population. There are different equations for the human health and the ecological indicators, because each has different types of data available and different requirements for comparing the effect of releases of TRI chemicals. Both human and ecological indicator elements incorporate estimates of the uncertainties associated with component weights. By using toxicity, exposure potential, and population size adjustments to the emission, the changes in the indicators over time should be more closely related to changes in risk than changes in emission quantities alone. It must be reiterated that while the resulting indicators are intended to relate to risk by considering toxicity, exposure and population factors, the indicators do not provide actual risk estimates.

The toxicity and exposure factors that are used to adjust the releases are referred to as weights. Briefly, the weights used to construct the TRI Environmental Indicators are derived by classifying a release in terms of ranges of toxicity, exposure, and population exposed, and assigning a weight value to each range. The weight assigned to each range increases as toxicity or exposure increase. The methodology for deriving weights is discussed in more detail below.

Several offices within the EPA and organizations outside the Agency have developed systems for scoring or weighting chemicals based on potential toxicity and exposure. The usual purpose of such exercises is to prioritize chemicals for further study or for closer regulatory scrutiny. A review of chemical scoring and ranking procedures used by offices within the Agency and by organizations outside the Agency is found in Appendix A.



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Previous scoring systems have used a variety of methods to weight chemicals. The actual numerical weights applied to chemicals can be qualitative, ordinal, weighted or calculated, or some combination of these approaches. The relative severity of the effects posed by chemicals can also be included, as can considerations of the quality of the toxicity data and the exposure estimates. Based on our review of these scoring systems, several options for a chemical evaluation methodology emerged. Alternative methods, and their advantages and disadvantages, were considered by the TRI Indicator Work Group and are summarized in Appendix B. The following section presents a proposed methodology based on the research described in Appendices A and B and based on Work Group deliberations. While the method described below contains elements of the options described in Appendix B, the draft methodology combines these elements in a manner that is not presented explicitly in the appendix.

**General Format of the Weighting Scheme**

Each TRI chemical will fall into one range of values for parameters of interest and will receive the corresponding weight based upon its characteristics. The methodology follows this categorization approach for both toxicity weighting and exposure weighting. A chemical may cause toxic effects to more than one health endpoint; thus, different weights could be assigned, depending on the endpoint considered. For this method, a chemical's final toxicity weight will be the highest weight it receives among all endpoints considered (i.e., based on its most sensitive endpoint).

Using categorical weights for toxicity and exposure has several advantages when compared to calculating specific, unique numerical weights for chemical releases. First, unique weights would imply that we know the toxicity and exposure potential of the release with enough precision to distinguish among relatively small differences in these values. In fact, there are significant uncertainties associated with both the toxicity data and the methods used to evaluate exposure potential. Weighting a release based on the broad categories of toxicity and exposure potential into which it falls avoids the impression of precision where such precision does not exist. Second, chemicals are likely to remain in the broad toxicity category to which they are originally assigned, unless significant new and different toxicity data become available. Thus, the weights applied to these chemicals are not likely to be revised frequently, lending stability to the indicators over time.

The following sections describe the methods used for toxicity and exposure weighting in both the human health and ecological TRI indicator calculations. The penultimate section describes rules for using the size of the exposed population in the TRI human health indicator calculation. The final section proposes a method for integrating the exposure, toxicity, and, where appropriate, population values in the TRI indicators calculations.



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## Toxicity Weights -- Human

For both carcinogenic and noncarcinogenic chronic effects, the proposed methodology for developing human health toxicity weights is based on scoring systems that include both qualitative and quantitative elements. There is uncertainty inherent in determining the potency of chemicals in causing human health effects, thus any quantitative potency data must be considered in the context of a qualitative classification of the uncertainty associated with that data. Therefore, the toxicity of each chemical is classified both quantitatively using potency data and qualitatively using weight-of-evidence (WOE). Both kinds of data are considered when deriving the score, and so both kinds of data must be generated for the TRI chemicals.

The Section 313 criteria list several human toxicity parameters that EPA must consider when evaluating a chemical for addition to TRI, including carcinogenicity, chronic toxicity, acute toxicity, reproductive toxicity, heritable gene and chromosomal mutations, developmental toxicity, and neurotoxicity. These parameters are defined in Table 8. A release could be weighted based upon the number of these effects that it causes, the relative severity of the effects it causes, and/or the potency of the chemical. Some chemicals have toxicity data for only one effect, while others will have evidence of effects for several of these toxicity categories. The following describes how available data on the toxicity of TRI chemicals will be used to weight releases.

### Quantitative Data Used in Human Toxicity Weighting

Quantitative data on the relative potencies of chemicals are needed for toxicity weighting. For cancer risk assessment, EPA has developed standard methods for predicting the incremental lifetime risk of cancer per dose of a chemical. EPA generally uses a linearized multistage model of carcinogenesis to quantitatively model the dose-response function of a carcinogen. The upper bound of the linear term of this model is called the $q_1^*$. This slope factor is a measure of cancer potency[1].

For noncarcinogenic risks, data on dose-response are more limited; generally, the assessor evaluates dose compared to a Reference Dose. A Reference Dose is defined as "an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime" (EPA, 1987c). By definition, exposures below this value are unlikely to produce an adverse effect; above this value, an exposed individual may be at risk for the effect, but the probability of the effect is not

[1] Although the level of conservatism inherent in these potency factors varies by chemical, $q_1^*$s nonetheless are the best readily available values that allow us to compare the relative potency of chemicals.



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## TABLE 8. Toxicity Endpoints

| Endpoint | Definition |
|---|---|
| Carcinogenicity | This toxicity concerns the ability of a chemical to produce cancer in animals or humans. |
| Heritable Genetic and Chromosomal Mutation | Chemicals which affect this endpoint can cause at least three separate modes of failure to transmit genetic information: gain or loss of whole chromosomes (aneuploidization), rearrangement of parts of chromosomes (clastogenesis), and addition or deletion of a small number of base pairs (mutagenesis). |
| Developmental Toxicity | Any detrimental effect produced by exposures to developing organisms during embryonic stages of development, resulting in: prenatal or early postnatal death, structural abnormalities, altered growth, and functional deficits (reduced immunological competence, learning disorders, etc.). |
| Reproductive Toxicity | This endpoint concerns the development of normal reproductive capacity. Chemicals can affect gonadal function, the estrous cycle, mating behavior, conception, parturition, lactation, and weaning. |
| Acute Toxicity | Acute toxicity indicates the potential for a short-term exposure (typically hours or days) by inhalation, oral, or dermal routes to cause acute health effect or death. |
| Chronic Toxicity | Chronic toxicity indicates the potential for any adverse effects other than cancer observed in humans or animals resulting from long-term exposure (typically months or years) to a chemical. |
| Neurotoxicity | This endpoint concerns the central and/or peripheral nervous system. Changes to the system may be morphological (biochemical changes in the system or neurological diseases) or functional (behavioral, electrophysiological, or neurochemical effects). |

known, nor is the severity of the effect known. For our purposes, we will assume that noncancer risk varies as the ratio of the estimated dose to the Reference Dose.

We have compiled human health effects data on the TRI chemicals from a number of EPA sources. Appendix C contains tables of available toxicity data for the TRI chemicals. The primary source of these toxicity data was the Integrated Risk Information System (IRIS). This computerized data source includes information on EPA evaluations of chemical toxicity for both carcinogens and noncarcinogens. IRIS provides both background information on the studies used to develop the toxicity evaluations and the numerical toxicity values used by EPA to characterize risks from these chemicals. These values include upper-bound cancer potency estimates ($q_1^*$) and Reference Doses (RfDs) for noncarcinogens and some carcinogens. Data contained in IRIS have been peer-reviewed and represent accepted Agency policy. It should be noted that this table contains health effects data for certain classes of metal compounds. These data represent the health effects data for the parent element, or, where appropriate, the health data of the most potent compound included in that category. To be conservative, the releases associated with these compound categories will be weighted based on these health effects data.

Another source of toxicity data is the Health Effects Assessment Summary Tables. These tables are constructed for use in both the Superfund program and in the RCRA Program but do not represent Agency consensus. However, these tables are publicly available in the Superfund docket. They also include potency estimates, WOE categorizations for carcinogens, and Reference Doses for noncarcinogens.

The Superfund program also develops reportable quantities that quantify the relative toxicity of chemicals. The Reportable Quantity (RQ) of a chemical is the minimum quantity of a release that requires immediate notification to the National Response Center by any person operating a vessel or facility. Separate reportable quantities are developed for several toxicity measures, including carcinogenicity, acute human toxicity, chronic human toxicity, and aquatic toxicity. RQs are also developed based on ignitability and reactivity. The regulatory RQ is then the lowest among these RQ values. For cancer, the reportable quantity value is assigned based on a combination of potency and WOE considerations. For the purposes of deriving the RQ, potency is characterized by the chemical's $ED_{10}$ value for cancer. The $ED_{10}$ is the dose that increases a response 10 percent above the control group (in this case, the response is cancer). Where specific potency data are not available, EPA scientists use guidelines provided in the RQ development methodology as well as best professional judgment to evaluate potential carcinogenic potency. For noncarcinogens, the RQ is based on an evaluation of the human-equivalent minimum effective dose (MED) and the severity of the effect produced at that dose. (The minimum effective dose is derived from the Lowest Observable Adverse Effect Level (LOAEL), with adjustments for nonchronic exposure and interspecies extrapolation).



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RQs, RfDs, and $q_1^*$s are all toxicity measures that have been developed for EPA risk evaluation purposes. One or more of these values are available for 247 TRI chemicals. The 70 TRI chemicals for which there are currently no formal EPA toxicity evaluations are found in Table 4. For these chemicals, potential toxicity will be evaluated based on toxicity data available from other data sources. These sources are listed in Appendix D. These sources, as well as quantitative structure activity relationship methods, may have to be used to supplement the formal available EPA toxicity values. For certain chemicals of extraordinary interest, special resources may have to be made available to perform an adequate toxicity evaluation. Chemicals for which little toxicity if any data exist, and thus no evaluation of toxicity is possible, will be excluded from the indicator calculation.

Qualitative Data Used in Human Toxicity Weighting

For toxicity weighting, the proposed method uses both weight of evidence (WOE) and potency to assign numerical toxicity weights. Typically, risk assessors use a variety of data to evaluate the potential toxicity of a chemical to humans, including epidemiological data, data from acute and chronic animal studies, and in vitro toxicity tests. Together, these data form a body of evidence regarding the potential for toxic chemicals to cause a particular health effect in humans. The risk assessor can qualitatively judge the strengths of this body of evidence when determining the probability of the occurrence of the effect in humans. Based on this judgment, the chemical is assigned a WOE classification. Weight-of-evidence schemes can be designed to demonstrate that a chemical causes a specific health effect in general, or specifically in humans. The categories for carcinogens are related to likelihood of effects in humans.

Standard weight-of-evidence classification schemes are widely used in cancer risk assessment. The carcinogenic WOE system presented in this methodology relies primarily on categorical definitions from two weighting/scoring systems: the EPA Cancer Risk Assessment Guidelines (EPA, 1986a, currently being revised) and the TSCA Chemical Scoring System (O'Bryan and Ross, 1988). The EPA Cancer Risk Assessment Guidelines define the following WOE categories:

| Category | Weight of evidence |
|---|---|
| A | Sufficient evidence from epidemiological studies to support a causal relationship between exposure to the agent and cancer. |
| B1 | Limited evidence from epidemiological studies and sufficient animal data. |
| B2 | Sufficient evidence from animal studies but inadequate or no evidence or no data from epidemiological studies. |



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| | |
|---|---|
| C | Limited evidence of carcinogenicity in animals and an absence of data or evidence in humans. |
| D | Inadequate human and animal evidence for carcinogenicity or no data. |
| E | No evidence for carcinogenicity in at least two adequate animal tests in different species or in both adequate epidemiological and animal studies, coupled with no evidence or data in epidemiological studies. |

The TSCA Chemical Scoring System also provides specific criteria for placing chemicals in toxicity categories based on WOE. This system can serve as a supplement to the EPA Risk Assessment Guidelines WOE categories. The TSCA Chemical Scoring System oncogenicity weight-of-evidence scoring system is similar to the categories in the EPA Cancer Risk Assessment Guidelines:

| Category | Weight of evidence |
|---|---|
| 8-9 | Evidence of oncogenicity from epidemiological studies and/or positive results in two or more mammalian species. |
| 6-7 | Evidence of oncogenicity in either or both sexes of a single mammalian species, with or without limited epidemiological data. |
| 4-5 | Suggestive evidence of oncogenic potential from epidemiological studies, mammalian bioassays, cell transformation in vitro, or promoter/cocarcinogenic activity. |
| 3 | Evidence of genotoxic potential. |
| 1-2 | Limited evidence of lack of oncogenic potential. |
| 0 | No evidence of oncogenic potential from well-conducted, well-designed mammalian studies in two or more animal species. |

These categories could be further modified to include a category of no evidence, similar to Group D, above. Many TRI chemicals have already been evaluated using one or both of these two schemes. Furthermore, there is ongoing work between OPPT and the Oak Ridge National Laboratory (ORNL) to score additional chemicals using this system. Therefore, the WOE evaluations using these two schemes are currently available for many TRI chemicals, and more will be available in the near future.

For noncarcinogens, WOE is routinely considered by EPA risk assessors when developing Reference Doses (RfDs). Reference Doses are usually developed based on a



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No Observable Adverse Effect Level (NOAEL) or a Lowest Observable Adverse Effect Level (LOAEL) combined with uncertainty factors and a modifying factor. The uncertainty factors are applied to account for (a) extrapolating from animal species to human populations, (b) extrapolating from less than chronic NOAELs to chronic NOAELs, and (c) extrapolating from studies on particular human populations to the general human population, including sensitive subpopulations. In addition, a modifying factor can be applied to reflect EPA's best professional judgment on the quality of the entire toxicity database for the chemical. Since EPA Reference Doses already include both uncertainty factors and a modifying factor based on deficiencies in the database, they require no further consideration of uncertainty in this methodology.

Unfortunately, EPA Reference Doses have not been developed for all TRI chemicals. When necessary, this methodology will require the evaluation of literature data to assign a toxicity weight to a chemical. In these circumstances, the following weight-of-evidence guidelines from the TSCA Chemical Scoring System can be used for the qualitative evaluation of the literature data:

For genotoxicity:

| Category | Weight of evidence |
|---|---|
| 9 | Evidence of mammalian mutagenicity/clastogenicity, interaction with mammalian germ cell DNA, or epidemiological data suggesting genotoxicity in humans. |
| 8 | Evidence of genotoxicity in nonmammalian germ cell assays, or evidence of mammalian dominant lethality. |
| 5-7 | Evidence of genotoxicity in more than one test system, other than above. |
| 2-4 | Limited evidence of genotoxicity, including mixed positive and negative results. |
| 1 | Limited evidence of nongenotoxicity. |
| 0 | Negative test results indicating lack of known genotoxicity. |



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For developmental effects:

| Category | Weight of evidence |
|---|---|
| 8-9 | Evidence of adverse developmental effects in humans or in at least two other mammalian species |
| 6-7 | Evidence of adverse developmental effects in one mammalian species. |
| 5 | Developmental effects at doses accompanied by maternal toxicity or otherwise equivocal test results. |
| 4 | Adverse developmental effects in nonmammalian species or in vitro test systems. |
| 3 | Indirect evidence suggesting possible adverse developmental effects. |
| 2 | Indirect evidence of lack of adverse developmental effects. |
| 1 | Limited evidence of lack of developmental effects. |
| 0 | No evidence of developmental toxicity potential. |

Again, categories for no evidence could be added to these scoring systems. EPA has also developed guidelines for certain noncarcinogenic effects. These guidelines can be used in conjunction with the TSCA Chemical Scoring System for qualitatively evaluating literature toxicity data on non-carcinogens. Guidelines for mutagenicity risk assessment (EPA, 1986b) describe general categories for WOE of mutagenicity, to which we have assigned letters for the purposes of this methodology:

For mutagenicity:

| Category | Weight of evidence |
|---|---|
| A | Positive data derived from human germ cell mutagenicity studies. |
| B | Valid positive results from studies on heritable mutation events in mammalian germ cells. |
| C | Valid positive results from mammalian germ cell chromosome aberration studies that do not include an intergeneration test. |



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| | |
|---|---|
| D | Sufficient evidence for a chemical's interaction with mammalian germ cells, together with valid positive mutagenicity test results from two assay systems. |
| E | Suggestive evidence for a chemical's interaction with mammalian germ cells, together with valid positive mutagenicity evidence from two assay systems. |
| F | Positive mutagenicity test results of less strength than defined in D, combined with suggestive evidence for a chemical's interaction with mammalian germ cell. |
| G | Valid negative test results for all endpoints of concern. |
| H | Inadequate evidence bearing on either mutagenicity or chemical interactions with mammalian germ cells. |

The Agency's "Proposed Amendments to the Guidelines for the Health Assessment of Suspect Developmental Toxicants" (EPA, 1989) delineates its categories with roughly the same criteria as that of the TSCA Chemical Scoring System.

To implement this method, similar weighting systems will need to be developed for neurotoxicity, reproductive toxicity and other chronic toxicity endpoints. The TSCA Chemical Scoring System defines scoring criteria for subchronic/chronic toxicity as a function of both a "severity score" and a "dose score." These criteria are:

| Severity score | Severity of effects |
|---|---|
| 3 | Life-threatening or severe effects |
| 2 | Moderately serious effects |
| 1 | Mild effects |
| 0 | No observed effects |

| Dose score | Effects | Guidelines |
|---|---|---|
| 3 | At low doses | <5 mg/kg-day |
| 2 | At intermediate doses | 5-50 mg/kg-day |
| 1 | At high doses | >50 mg/kg-day |

These criteria can be adopted and/or modified for use in this methodology.



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General Format for Combining Weight of Evidence and Potency

This methodology uses matrices to evaluate a chemical based on WOE and potency simultaneously. Rows and columns form matrix cells to which a toxicity weight is assigned. The rows of the matrix are defined by the weight-of-evidence categorization, while the columns of the matrix are defined by ranges of the measure of cancer potency (such as $q^*$) or the measure of noncarcinogenic threshold doses (such as NOAELs). More than one kind of quantitative measure can be used to weight chemicals. By taking advantage of a range of data sources available to weight chemicals, more TRI chemicals can be weighted and included in the indicator. For example, for the cancer potency, one chemical may have a $q_1^*$ value, while another chemical may have only an $ED_{10}$ value. The toxicity weighting matrix for cancer is constructed so that either measure can be used to assign a weight. If both measures are available, the value that results in a higher weight will be used. The heading of a matrix column reflects the range of values that fall into that column. Ranges of different toxicity measures that appear in the same column heading reflect a roughly comparable magnitude of toxicity. Similarly, WOE descriptions appearing in the same row label represent roughly the same category of WOE.

The exception to this weighting format is chemicals for which RfDs are available. As discussed above, WOE is considered in the development of RfDs and is already incorporated in the numerical value. Therefore, the matrix approach is unnecessary. For these chemicals, weights will be applied based on ranges of RfD values alone.

Weights Applied to the Categories

Either ordinal or proportional weights could be assigned to the matrix cells. Ordinal weights delineate the relative toxicity rank among releases and are useful for setting priorities. They do not, however, provide information on the magnitude of the toxicity of chemicals relative to one another. For example, an ordinal rank of 3 for chemical A and 1 for chemical B does not mean chemical A is three times worse than chemical B. Since ordinal weights do not reflect proportional differences in toxicity, the ability of the indicator to reflect changes in health and environmental impacts could be limited if ordinal weights are used. In fact, if ordinal weights are used, it is possible that the indicator could decrease over a period when actual risk increases. An example of this possibility is illustrated in Figure 2.

Unlike ordinal systems, proportional scoring systems use numerical scores that reflect the magnitude of difference between the impacts associated with chemical releases. Figure 3 shows how the indicator value developed in Figure 2 would change if proportional rather than ordinal weights are assigned to the categories. Because of these considerations, the matrices used in this methodology assign proportional weights to matrix cells. Weights increase by an order of magnitude for each order of magnitude increase in toxicity and for each increase in WOE category.



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Figure 2

Assume that the following scoring system is used to calculate the TRI indicator. The indicator traces the releases of carcinogens to air:

| $q_1^*$ Value | Exposure (mg/kg-day) | Score |
|---|---|---|
| 50 or greater | greater than 50 | 6 |
| 5<x<50 | 5-50 | 5 |
| 0.5<x<5 | 0.5-5 | 4 |
| 0.05<x<0.5 | 0.05-0.5 | 3 |
| 0.005<x<0.05 | 0.005-0.05 | 2 |
| 0.0005<x<0.005 | 0.0005-0.005 | 1 |
| less than 0.0005 | less than 0.0005 | 0 |

Component scores are calculated by multiplying the toxicity ranking (the $q_1^*$ ranking) by the exposure ranking and by the exposed population. The result is divided by 100,000 to eliminate unnecessary orders of magnitude.

Assume that the TRI set of chemicals and facilities consists of two chemicals and two facilities. We have the following data:

| Year | Plant | Chemical | $q_1^*$ (kg-day/mg) | Population Exposed | Exposure Level (mg/kg-day) | Estimated Cases |
|---|---|---|---|---|---|---|
| 1 | 1 | vinyl chloride | 2.3 | 100,000 | 0.006 | 1,380 |
| 1 | 2 | benzene | 0.029 | 1,000,000 | 0.006 | 174 |
| 2 | 1 | vinyl chloride | 2.3 | 100,000 | 0.08 | 18,400 |
| 2 | 2 | benzene | 0.029 | 1,000,000 | 0.003 | 87 |



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The corresponding scores would be:

| Year | Plant | Chemical | Toxicity Score | Population Score | Exposure Score | Overall Score |
|---|---|---|---|---|---|---|
| 1 | 1 | vinyl chloride | 4 | 100,000 | 2 | 8 |
| 1 | 2 | benzene | 2 | 1,000,000 | 2 | 40 |
| 2 | 1 | vinyl chloride | 4 | 100,000 | 3 | 12 |
| 2 | 2 | benzene | 2 | 1,000,000 | 1 | 20 |

The overall TRI indicator for year one is 48, while for year two it is 32. Thus, from the indicator, it would appear as if health risks have decreased. However, the acutal number of expected cancer cases has increased dramatically, from roughly 1,600 to over 18,500.



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Figure 3

Assume that the following scoring system is used to calculate the TRI indicator. The indicator traces the releases of carcinogens to air:

| $q_1^*$ Value | Exposure (mg/kg-day) | Score |
|---|---|---|
| 50 or greater | greater than 50 | 1,000,000 |
| 5<x<50 | 5-50 | 100,000 |
| 0.5<x<5 | 0.5-5 | 10,000 |
| 0.05<x<0.5 | 0.05-0.5 | 1,000 |
| 0.005<x<0.05 | 0.005-0.05 | 100 |
| 0.0005<x<0.005 | 0.0005-0.005 | 10 |
| less than 0.0005 | less than 0.0005 | 1 |

Component scores are calculated by multiplying the toxicity ranking (the $q_1^*$ ranking) by the exposure ranking and by the exposed population. The result is divided by $1 \times 10^9$ to eliminate unnecessary orders of magnitude.

Assume that the TRI set of chemicals and facilities consists of two chemicals and two facilities. We have the following data:

| Year | Plant | Chemical | $q_1^*$ (kg-day/mg) | Population Exposed | Exposure Level (mg/kg-day) | Estimated Cases |
|---|---|---|---|---|---|---|
| 1 | 1 | vinyl chloride | 2.3 | 100,000 | 0.006 | 1,380 |
| 1 | 2 | benzene | 0.029 | 1,000,000 | 0.006 | 174 |
| 2 | 1 | vinyl chloride | 2.3 | 100,000 | 0.08 | 18,400 |
| 2 | 2 | benzene | 0.029 | 1,000,000 | 0.003 | 87 |



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The corresponding scores would be:

| Year | Plant | Chemical | Toxicity Score | Population Score | Exposure Score | Overall Score |
|---|---|---|---|---|---|---|
| 1 | 1 | vinyl chloride | 10,000 | 100,000 | 100 | 100 |
| 1 | 2 | benzene | 100 | 1,000,000 | 100 | 10 |
| 2 | 1 | vinyl chloride | 10,000 | 100,000 | 1,000 | 1,000 |
| 2 | 2 | benzene | 100 | 1,000,000 | 10 | 1 |

Using proportional weighting, the overall TRI indicator for year one is 110, while for year two it is 1,001. Thus the increase in risk protrayed by the indicator successfully reflects the increase in the estimated number of cancer cases.



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The Human Health Toxicity Matrices

The preceding discussion presented the general framework for weighting the toxicity of TRI releases. This section describes and explains the matrices developed from this framework. Two separate toxicity weighting matrices for carcinogens and noncarcinogens are discussed.

Carcinogens. The toxicity weighting matrix for carcinogens is found in Figure 4. The rows of the matrix qualitatively classify carcinogens into two general categories: known/probable and possible. Weight-of-evidence categories A, B1 and B2 of the EPA Cancer Risk Assessment Guidelines and categories 6-9 of the TSCA Chemical Scoring System cancer WOE scheme are placed in the "known/probable" category. Class C carcinogens and TSCA Chemical Scoring categories 3-5 are placed in the "possible" category.

The columns of the matrix describe quantitative measures of toxicity. Two alternative measures are presented: the EPA $q_1^*$ and the $ED_{10}$. Furthermore, the development methodology for cancer RQs (EPA, 1988a) provides criteria for assigning a chemical to a potency group in the absence of an $ED_{10}$; these criteria can be used for approximating the range of the $ED_{10}$ for purposes of chemical weighting in the current methodology. The particular ranges of $q_1^*$ values selected to represent each category of cancer potency were chosen to correspond to the ranges presented in EPA's Hazard Ranking System (55 Federal Register 51532). (Corresponding ranges for comparable $ED_{10}$ values will need to be developed.) The Hazard Ranking System (HRS) is a multipathway scoring system "used to assess the threat associated with actual or potential releases of hazardous substances at sites" (Federal Register, *op cit.*). The HRS score determines whether a site will be included on the National Priorities List (NPL). Part of the HRS scoring system rates the inherent toxicity of chemicals based on measures of cancer potency, RfDs, and/or acute toxicity. Ranges of toxicity values that differ by an order of magnitude are assigned scores that differ by an order of magnitude. The actual numerical weights assigned to the matrix cells in Figure 4 correspond to the scores assigned in the HRS to these ranges. In certain cases, ranges presented in our matrix extend beyond those presented in the HRS. However, the basic logic of assigning the weights to these ranges remains the same: ranges that differ by an order of magnitude are assigned weights that differ by an order of magnitude. Figure 5 shows the distribution of $q_1^*$ values in these ranges for the TRI chemicals that have these values.

The cells in the first row of the matrix (that is, the row that corresponds to the "known/probable" WOE category) were assigned the weights based on the HRS values. Weights in the lower row (i.e., the lower WOE category) were assigned by dividing the weights in the row above by a factor of 10.

## Figure 4. Toxicity Weighting Matrix for Carcinogens

| WEIGHT OF EVIDENCE | | | POTENCY CATEGORY | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| General Category | EPA Risk Assessment Guidelines Category | TSCA Chemical Scoring System Category | <0.005 | 0.005–0.05 | 0.05–0.5 | 0.5–5 | 5–50 | >50 | ED10 EPA $q_1^*$ Value |
| Known/Probable | A/B | 6–9 | 10 | 100 | 1000 | 10000 | 100000 | 1000000 | |
| Possible | C | 3–5 | 1 | 10 | 100 | 1000 | 10000 | 100000 | |

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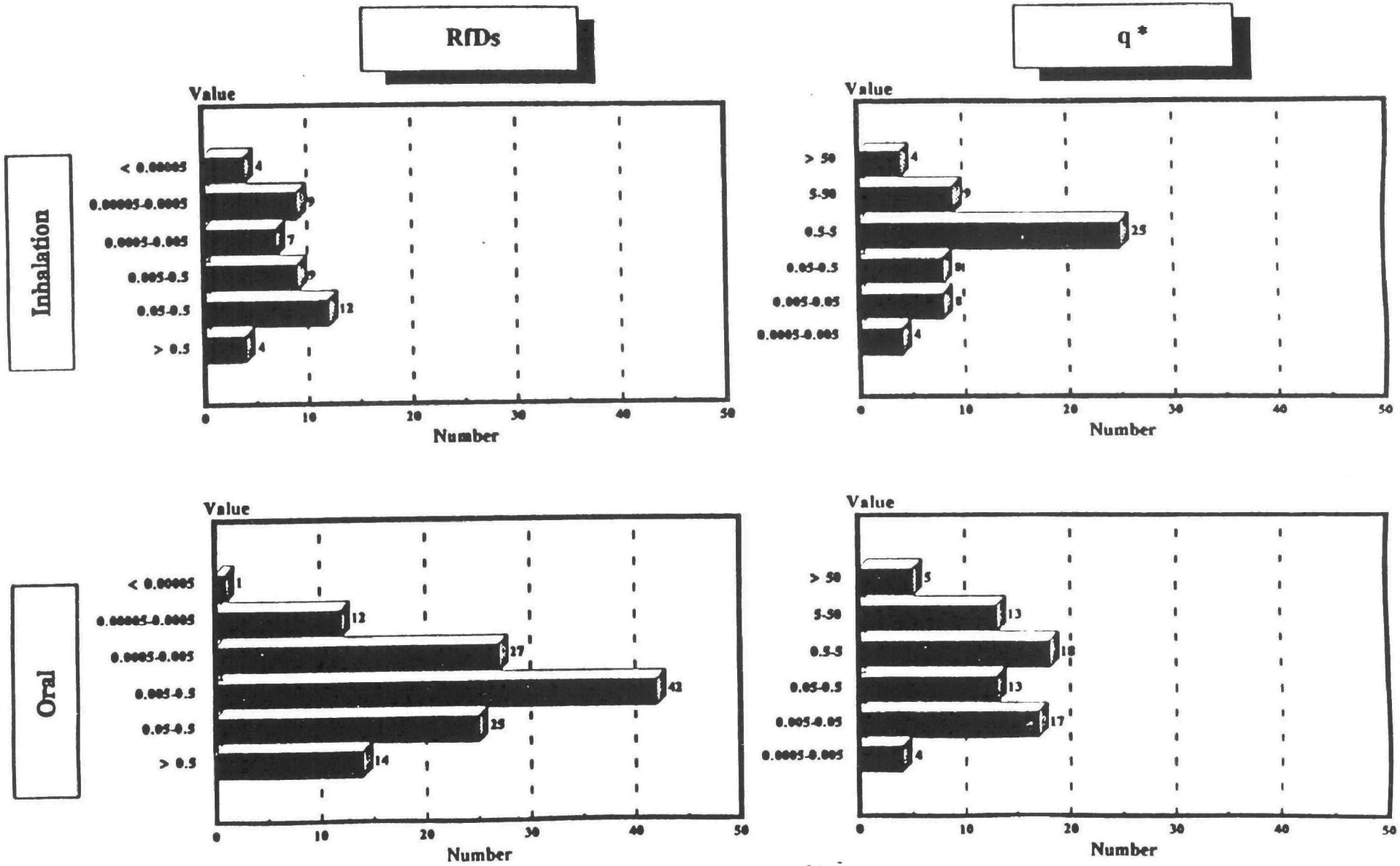
# Figure 5
# Distribution of Toxicity Values



Noncarcinogens. For noncarcinogens that have established RfDs, the following toxicity weights will be used:

| RfD Range (mg/kg-day) | Assigned Weight |
|---|---|
| RfD < 0.00005 | 100,000 |
| 0.00005 < RfD< 0.0005 | 10,000 |
| 0.0005 < RfD < 0.005 | 1,000 |
| 0.005 < RfD < 0.05 | 100 |
| 0.05 < RfD < 0.5 | 10 |
| 0.5 < RfD | 1 |

This weighting system is taken directly from the HRS, with the exception of the highest weighting category. The weight assigned to this category is logically consistent with the HRS scoring system: RfDs less than 0.00005 are assigned a weight that is an order of magnitude greater than RfDs between 0.00005 and 0.0005. Figure 5 shows the distribution of RfD values in all of these ranges for those TRI chemicals that have RfDs.

For noncarcinogens without RfDs, a toxicity weighting matrix is presented, as shown in Figure 6. The rows of this matrix also qualitatively classify WOE into two general categories: known/probable and possible. Categories 5-9 of the TSCA Chemical Scoring System WOE schemes for noncarcinogens are placed in the "known/probable" category, and categories 2-4 are placed in the "possible" category. For mutagens, EPA mutagen risk assessment guideline categories A-E are placed in the "known/probable" category and F in the "possible" category.

The columns of this matrix are labeled with the numerical ranges of values that define each category of noncancer toxicity. Measures that can be used to quantitatively weight toxicity include the human-adjusted NOAEL (the No Observable Adverse Effect Level), human-adjusted Lowest Observable Adverse Effect Level (LOAEL), and the human-adjusted minimum effective dose (MED). The ranges for the NOAEL values are defined to roughly correspond to the ranges of RfDs presented above. Corresponding ranges for LOAEL and MED values still must be developed.

The cells in the first row of the matrix (that is, the row that corresponds to the "known/probable" WOE category) were assigned the same weights as those assigned to the RfD ranges. Weights in the lower row (i.e., the lower WOE category) were assigned by dividing the weights in the row above by a factor of 10.

Selecting the Final Human Health Toxicity Weight for a Chemical

Chemicals can cause several types of toxic effects. The TRI Human Health Chronic Indicator method will weight a chemical based on the endpoint associated with the lowest dose at which an effect occurs. Under this regime, the same weights are assigned to similar

Figure 6. Toxicity Weighting Matrix for Noncarcinogens

| WEIGHT OF EVIDENCE | | | DOSE CATEGORY | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | MED (mg/kg-dy) |
| | | | | | | | | | LOAEL (mg/kg-dy) |
| General Category | EPA Risk Assessment Guidelines Category | TSCA Chemical Scoring System Category | 0.5 < | 0.05–0.5 | 0.005–0.05 | 0.0005–0.005 | 0.00005–0.0005 | <0.00005 | NOAEL (mg/kg-dy) |
| Known/Probable | A–E | 5–9 | 1 | 10 | 100 | 1000 | 10000 | 100000 | |
| Possible | F | 2–4 | 0.1 | 1 | 10 | 100 | 1000 | 10000 | |

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cells in each category of toxicity so that chemical toxicity scores are comparable across different types of toxic effects. For example, a highly potent genotoxin with strong WOE would get the same score as a highly potent carcinogen with strong WOE.[2]

The approach of weighting based on the endpoint with the lowest dose does not consider differences in the severity of the effects posed by the chemicals. For example, cancer is weighted in the same manner that genotoxicity is weighted. Also, chemicals with a broad range of effects are weighted the same as a chemical with only one effect. The TRI Indicator Work Group considered the option of applying an additional factor to the toxicity weight based on the severity of the effect. Applying such weights across categories of toxic endpoints would require a subjective evaluation of the relative severity of the health effects. The Work Group also considered the option of applying an additional weight based on the number of endpoints for which the chemical demonstrates effects. However, a chemical may appear to demonstrate just one effect only because there are no data on other effects; thus, applying a weight based on the number of endpoints may undervalue some poorly studied but still risky chemicals. For these reasons, the Work Group rejected these options; the methodology will weight chemicals based on the most severe endpoint without applying additional weights for severity or number of effects caused.

Toxicity Weights -- Ecological

For ecological effects, the indicator will focus on aquatic life impacts. Very little data are available for most chemicals on effects to terrestrial or avian species, and the human health indicator will provide some predictor of these.

Aquatic toxicity weighting differs from human toxicity weighting in two important respects. First, WOE is not considered a factor in the weighting scheme, since direct evidence of chemical toxicity is available from tests on aquatic species. Second, the aquatic toxicity weighting scheme simultaneously considers toxicity and bioaccumulation potential. Both of these measures are considered important when evaluating impacts on aquatic ecosystems.

Data Used in Aquatic Toxicity Weighting

Common numerical aquatic toxicity data include the Acute or Chronic Ambient Water Quality Criteria (AWQC), developed by the Office of Water, which may serve as the basis for water quality standards, as well as values from the literature, such as the lethal concentration, 50 percent ($LC_{50}$) - the chemical concentration in water at which 50 percent

[2]The toxicity weighting may be pathway-specific for chemicals that demonstrate different effects by different pathways. For example, some chemicals are carcinogens by the inhalation pathway, but not by ingestion. Thus, the toxicity weighting may be different for different release pathways.



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of test organisms die - or life-cycle or chronic No Observable Adverse Effect Levels (NOAELs). Aquatic RQ values are also available for some TRI chemicals; aquatic RQs are determined based on the aquatic $LC_{50}$ of the chemical. Appendix C lists the AWQC and aquatic RQs that have been developed for TRI chemicals. Additional aquatic toxicity data will be obtained from the Aquatic Toxicity Retrieval System (AQUIRE), an aquatic toxicity database maintained by EPA. These data will be reviewed by OPPT before use in the indicator.

The preferred measures of bioaccumulation potential are the bioconcentration factor (BCF) or bioaccumulation factor (BAF). These values are derived from laboratory tests that compare the contaminant concentration in the environmental medium to the concentration in the tissues of a test organism (usually fish). Several researchers have found that for organic contaminants, the BCF or BAF can be approximated as a function of the log of the octanol water partition coefficient (log $K_{ow}$). The $K_{ow}$ is a physicochemical property that describes the partitioning of organic chemicals between an organic solvent (octanol) and water. Finally, when neither of these measures are available, the bioaccumulation potential can also be approximated by the water solubility of the chemical. Generally, the less soluble a chemical, the greater its potential for bioaccumulation. Values for all of these measures of bioaccumulation potential are available from a variety of sources, including the AQUIRE database, as well as a number of EPA Office of Water references, the EED chemical properties data base and standard chemical reference books.

The Aquatic Toxicity Weighting Matrix

The aquatic toxicity weight assigned to a chemical is a function of both its aquatic toxicity values and bioaccumulation potential values. Separate weights are assigned based on each of these measures; the chemical's final toxicity weight is the product of these individual weights. The individual weights assigned based on the measures of bioaccumulation potential are the following:

| Water Solubility (mg/l) | Log Kow | BCF (l/kg) | Weight |
|---|---|---|---|
| > 1,500 | <0.8 | <1 | 0.5 |
| 500-1500 | 0.8-2 | 1-10 | 5 |
| 25-500 | 2-3.2 | 10-100 | 50 |
| - . | 3.2-4.5 | 100-1,000 | 500 |
| - | 4.5-5.5 | 1,000-10,000 | 5,000 |
| <25 | 5.5-6.0 | >10,000 | 50,000 |

Individual weights based on aquatic toxicity measures are the following:

| Life Cycle or Chronic NOAEL ($\mu$g/l) | $LC_{50}$ ($\mu$g/l) | Acute AWQC or AALAC ($\mu$g/l) | Chronic AWQC or AALAC ($\mu$g/l) | Weight |
|---|---|---|---|---|
| >100 | >1,000 | >100,000 | >1,000 | 1 |
| 10-100 | 100-1,000 | 10,000-100,000 | 100-1,000 | 10 |
| 1-10 | 10-100 | 1000-10,000 | 10-100 | 100 |
| 0.1-1 | 1-10 | 100-1,000 | 1-10 | 1,000 |
| <0.1 | <1 | <100 | <1 | 10,000 |

As with the human health toxicity weighting, the quantitative measures used to represent aquatic toxicity, the value ranges used to define the categories of toxicity, and the numerical weights assigned to each category were for the most part taken from the Hazard Ranking System. The only exception is the ranges for life cycle or chronic NOAELs, which were taken from the TSCA Chemical Scoring System.

Figure 7 presents the combined toxicity weighting system for aquatic toxicity. The rows of the matrix are defined by the bioaccumulation potential categories and the columns of the matrix are defined by the aquatic toxicity categories. The cells of the matrix are the product of the chemical's bioaccumulation potential and aquatic toxicity weights.

## Exposure Weights -- Human

As with toxicity weighting, both qualitative and quantitative elements are considered when weighting exposure potential. Three steps are involved in deriving the human exposure weight. The first step is to categorize some measure of exposure potential into numerical ranges. The second step is to categorize the levels of uncertainty associated with the measures of exposure potential. The final step uses a matrix, with numerical exposure potential ranges arrayed along one axis and uncertainty categories arrayed along the other, to assign increasing weights to higher-certainty/higher exposure potential releases.

### Quantitative Data Used in Exposure Potential Weighting

For the first step of this process, quantitative measures of exposure potential must be estimated. To do so, several existing scoring systems take the approach of ordinally ranking the volume of each release by the same physical measure of the chemical's ability to move through the environmental medium into which it is released. However, because the exposure potential rankings would have different physical meanings for different



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Figure 7. Aquatic Toxicity Matrix

| BIOACCUMULATION | | | AQUATIC TOXICITY CATEGORY (ug/l) | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | >100 | 10–100 | 1–10 | 0.1–1 | <0.1 | Life Cycle or Chronic NOAEL |
| Water Solubility (mg/l) | Log Kow | BCF (l/kg) | >1000 | 100–1000 | 10–100 | 1–10 | <1 | LC50 |
| | | | >100,000 | 10,000–100,000 | 1000–10,000 | 100–1000 | <100 | Acute AWQC or AALAC |
| | | | >1000 | 100–1000 | 10–100 | 1–10 | <1 | Chronic AWQC or AALAC |
| >1,500 | <0.8 | <1 | 0.5 | 5 | 50 | 500 | 5000 | |
| 500–1500 | 0.8–2 | 1–10 | 5 | 50 | 500 | 5000 | 50000 | |
| 25–500 | 2–3.2 | 10–100 | 50 | 500 | 5000 | 50000 | 500000 | |
| – | 3.2–4.5 | 100–1000 | 500 | 5000 | 50000 | 500000 | 5000000 | |
| – | 4.5–5.5 | 1000–10,000 | 5000 | 50000 | 500000 | 5000000 | 50000000 | |
| <25 | 5.5–6.0 | >10,000 | 50000 | 500000 | 5000000 | 50000000 | 500000000 | |

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pathways, comparisons among releases to different media would be difficult, and weighted releases from different pathways could not be added to obtain a single indicator value.

In this methodology, comparisons across media can be made because a common quantitative exposure measure for each medium is derived: an estimate of "surrogate dose" -- a measure related to the amount of chemical contacted by an individual per kg body weight per day. Although limited facility-specific data and the use of generic models (described below) prevent the calculation of an actual dose, the surrogate dose measure developed from the available data and from generic modeling is designed to be, in concept, comparable for all media.

To estimate the magnitude of exposure potential from TRI releases, a separate exposure evaluation is conducted for each release pathway. The ideal derivation of an exposure weight would involve a site-specific exposure assessment for each release medium and for each exposure pathway. However, such an effort is well beyond the scope of this project and well beyond the intended use of the TRI data. These data are frequently estimates of emissions, not precise measured values. Notably, they are not estimates of environmental concentrations that result from the emissions from the plant. Furthermore, extensive site-specific information relevant to exposure modeling is not part of a TRI data submission. For example, the TRI forms do not require submission of data on groundwater flow, soil conditions, and other factors that affect groundwater contamination from land releases. It is not the intent of this project to gather additional data or measurements that would be needed to perform these calculations. The need to accurately reflect exposure characteristics in the indicator must be balanced by the need for a simple and understandable indicator that is easily communicated to the public and that is based on currently available data. Therefore, for this methodology, the exposure evaluations combine data on media-specific emission volumes, physicochemical properties, and where available, site characteristics with site-specific or generic exposure models to determine an estimate of the ambient concentration of contaminant in the medium into which the chemical is released. (Again, the use of submitter-estimated TRI emission data and generic models with many default assumptions make this only a surrogate related to actual concentration). For the human health chronic indicator, the ambient media concentrations are then combined with standard human exposure assumptions to estimate the magnitude of the surrogate dose.

It must be emphasized that while this methodology uses the EPA exposure assessment paradigm to evaluate exposure potential, the results should not be construed as an actual absolute numerical estimate of dose resulting from TRI releases. Instead, the purpose is to obtain an order of magnitude estimate of surrogate dose resulting from release of TRI chemicals *relative to the surrogate dose resulting from other releases included in the indicator*, so that these releases can be weighted appropriately in the indicator.

The exposure evaluation methods used for each type of release are specific to that type of release and depend on the models and data available to evaluate that pathway. In some cases, models will be combined with some site-specific data to estimate exposure; in

other cases, generic worst-case models may be used in the absence of any site-specific data. Section V of this report presents an extensive discussion of the specific mechanisms for evaluating exposure for each type of release or transfer.

Qualitative Data Used in Exposure Potential Weighting

Consideration of uncertainty in the exposure evaluation is necessary for making comparisons across pathways, since the exposure evaluation methods for various pathways differ significantly in their possible level of refinement. For the purposes of exposure weighting, we have defined the following uncertainty categories for use in this methodology:

| Category | Explanation |
|---|---|
| A | Combines modeling with some generic and some dependable site-specific data to generate exposure estimates. |
| B | Combines modeling with some generic and some site-specific data, but identification of appropriate site-specific data subject to error and will often be filled in with generic assumptions. |
| C | Extrapolates generic exposure estimates from actual data from other sites to exposure at particular sites (e.g., groundwater modeling). |

In general, more generic methods for exposure modeling require more assumptions and extrapolations. These assumptions and extrapolations tend to be conservative, so that more generic modeling tends to yield overestimates of exposure. The categories defined above are designed so that a lower category indicates more generic modeling that is likely to overestimate exposure when compared to the next highest category.

The Human Exposure Potential Weighting Matrix

As with toxicity weighting, a matrix has been developed to weight exposure potential that allows simultaneous consideration of the estimated level of exposure and the evaluation of the relative level of uncertainty associated with each estimate. The matrix for exposure weighting is presented in Figure 8. The exposure value is expressed in mg/kg-day and is calculated on a pathway-specific basis, as described in Section V. The uncertainty categories are as defined above. As with toxicity weighting, proportional weights are assigned so that exposures that differ by an order of magnitude are assigned weights that differ by an order of magnitude.

As discussed above, the exposure uncertainty categories are designed so that a lower category indicates that the exposure estimate is probably an overestimate compared to the next highest category; therefore, for this methodology, the exposure potential score will be



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Figure 8. Exposure Weighting Matrix

| UNCERTAINTY CATEGORY | ESTIMATED EXPOSURE (mg/kg–day) | | | | | | |
|---|---|---|---|---|---|---|---|
| | <0.0005 | 0.0005–0.005 | 0.005–0.05 | 0.05–0.5 | 0.5–5 | 5–50 | >50 |
| A | 1 | 10 | 100 | 1000 | 10000 | 100000 | 1000000 |
| B | 0.2 | 2 | 20 | 200 | 2000 | 20000 | 200000 |
| C | 0.1 | 1 | 10 | 100 | 1000 | 10000 | 100000 |

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reduced by a factor of 5 if assigned to category B, and by an order of magnitude if assigned to category C.

Exposure Weights -- Ecological

The estimated ambient water concentration value is used directly to evaluate potential exposures to aquatic life. The method for evaluating ambient surface water concentrations resulting from TRI releases is discussed in Section V. Once ambient concentrations have been determined, exposure weights are assigned based on the following ranges:

| Estimated water concentration ($\mu g/l$) | Weight |
|---|---|
| < 1 | 1 |
| 1-10 | 10 |
| 10-100 | 100 |
| 100-1,000 | 1,000 |
| > 1000 | 10,000 |

Aquatic exposure weights for categories of increasing estimated water concentration do not need to reflect exposure relative uncertainty, since all estimates are derived using the same methodology. The weights simply increase by an order of magnitude for each category.

Population Size Weights

The Work Group considered several options for including population in the indicator. One suggestion was to represent populations as ranges rather than using absolute numbers, especially for small populations. Use of a range may be more appropriate given the uncertainty about the size of the exposed population for most exposure pathways. Another reason for this approach is to avoid undervaluing potentially high individual impacts on small rural populations. Using a range approach, small rural populations would be assured of a minimum weighting. On the other hand, if reliable population data are available, an argument can be may for avoiding the introduction of additional uncertainty in the indicator by using ranges for population values.

In light of these considerations, this methodology proposes several rules for the use of population data in the exposure evaluation. First, a minimum population value is assigned to all releases to avoid undervaluing rural populations. Second, both quantitative data and qualitative data (on the uncertainty of the population size estimate) are used when evaluating the size of the population potentially exposed to TRI releases.

Quantitative Data Used in Population Weighting

The determination of the size of the population exposed to TRI releases will vary substantially depending on the medium to which the chemical is released. The methods for estimating the size of the exposed population are discussed for each pathway in Section V.

Qualitative Considerations in Evaluating Exposed Population Size

Methods for estimating exposed population sizes will vary in their accuracy. We may have good data on the number of persons surrounding a particular release site but know little about how many of these individuals actually come into contact with contaminated media. The uncertainty associated with the population estimate will differ by pathway. For example, the size of the population potentially exposed to contaminated groundwater will be known with significantly less certainty than the size of the population exposed to air emissions, because of the greater certainty associated with air modeling (we know who lives around the sites, and everyone breathes air) than with modeling of groundwater (location and movement not known, number of persons drinking groundwater not known).

To address this concern, this methodology will consider uncertainty in the evaluation of the size of exposed populations. Uncertainty categories are defined as follows:

| | |
|---|---|
| A | Population size is well-characterized, and contact with contaminated media is believed to affect most or all members of the exposed population. |
| B | Population is characterized using crude data that is likely to overestimate size of exposed population, but contact with contaminated media is believed to affect most or all members of the exposed population. |
| C | Population is characterized using crude data that is likely to over estimate size of exposed population, and contact with contaminated media occurs with an unknown fraction of those potentially exposed. |

A lower category indicates that the population estimate is probably an overestimate compared to the next highest category; therefore, for this methodology, the estimated size of the population will be reduced by a factor of 10 if assigned to category B, and by two orders of magnitude if the population estimate is assigned to category C.

All population sizes will also be rounded up to the nearest 1,000 persons. By rounding, we acknowledge that the methods used to estimate the population sizes are imperfect and do not justify the use of precise values. Also, this rounding creates a minimum exposed population size, since populations of 0-999 persons will be counted as



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1000. A minimum population size ensures the inclusion of rural populations in the indicator.

Because of the major difficulties in estimating sizes of the populations of ecological receptors, the TRI Ecological Indicator does not include a population weight. In effect, this approach assumes that all aquatic emissions occur to equally vulnerable locations.

## Integrating Toxicity Data, Exposure Data, and Population Data to Obtain Facility-Chemical-Medium Indicator Elements

### Human Health Chronic Indicator

The previous sections described how each element of the human health chronic indicator is determined. The following equation combines these components for each facility, each chemical, and each medium:

$$Element_{ijk} = ToxicityWeight_{ij} \cdot ExposureWeight_{ijk} \cdot AdjustedPopulation_{jk}$$

where

| | | |
|---|---|---|
| $i$ | = | subscript for chemical i, |
| $j$ | = | subscript for facility j, and |
| $k$ | = | subscript for medium k. |

The weights and the population size are multiplied in this setting because each component (toxicity, exposure, and population) contributes in a multiplicative way to the overall magnitude of the impact. The result of the multiplication of the weights is a facility-chemical-medium-specific "indicator element." It must be reiterated that this is not a physically meaningful measure of risk associated with the facility, but is an approximate measure that is comparable to approximate measures for other facilities calculated using the same methods. In Section VI, these elements will be combined into a single TRI chronic human health indicator. These elements can be used for diagnostic purposes when the indicator is calculated.

### Ecological Chronic Indicator

The methods for determining aquatic toxicity and exposure weights are described above. The following general equation combines these components for each facility, each chemical, and each medium:

$$Element_{ijk} = ToxicityWeight_{ij} \cdot ExposureWeight_{ijk},$$

where
$i$ = subscript for chemical i,
$j$ = subscript for facility j, and
$k$ = subscript for medium k.

As with the human health indicator, the weights are multiplied in this setting because each component (toxicity and exposure) contributes multiplicatively to the overall magnitude of the impact. The result of the multiplication of the weights is a facility-chemical-medium-specific "indicator element." Again, the elements should not be interpreted as actual measures of risk. In Section VI, these elements will be combined into a single TRI chronic ecological indicator.

## V. MECHANICS OF ESTIMATING EXPOSURE

The preceding section addressed how exposure and toxicity will be assigned weights based on the relative magnitude of each and the underlying uncertainty. The purpose of this section is to describe how the magnitude of exposure is calculated for each pathway. Ideally, we would model each TRI release with the rigor of a full risk assessment, relying on site-specific data. This is impossible, however, because resources and information are limited. For a set of indicators that are meant to generally track relative year to year changes in human and environmental health impacts, it is also unnecessary. For our purposes, it is adequate to approximate the results of such a modeling exercise.

TRI chemical releases are reported for seven different release and transfer pathways. On-site pathways include direct air (stack and fugitive), landfilling, underground injection, and surface water releases. Chemicals might also be transferred to Publicly Owned Treatment Works (POTWs) or Treatment, Storage, and Disposal Facilities (TSDFs). The release and transfer pathways for which exposure potential must be evaluated are presented in Figure 9.

To incorporate exposure in the TRI indicators, the TRI Indicator Work Group considered two fundamental approaches. First, releases could be weighted using proxy measures of exposure, such as population density surrounding the facility, and/or environmental mobility characteristics. Alternatively, releases could be modeled, where possible, to derive ambient environmental concentrations of contaminants at varying distances from the release site, and then combined with the corresponding population data.

When considering modeling versus a more simplified approach, the Work Group noted the fact that some releases (such as air releases) may be more amenable to a modeling approach than other types of releases (such as offsite transfers); thus, releases

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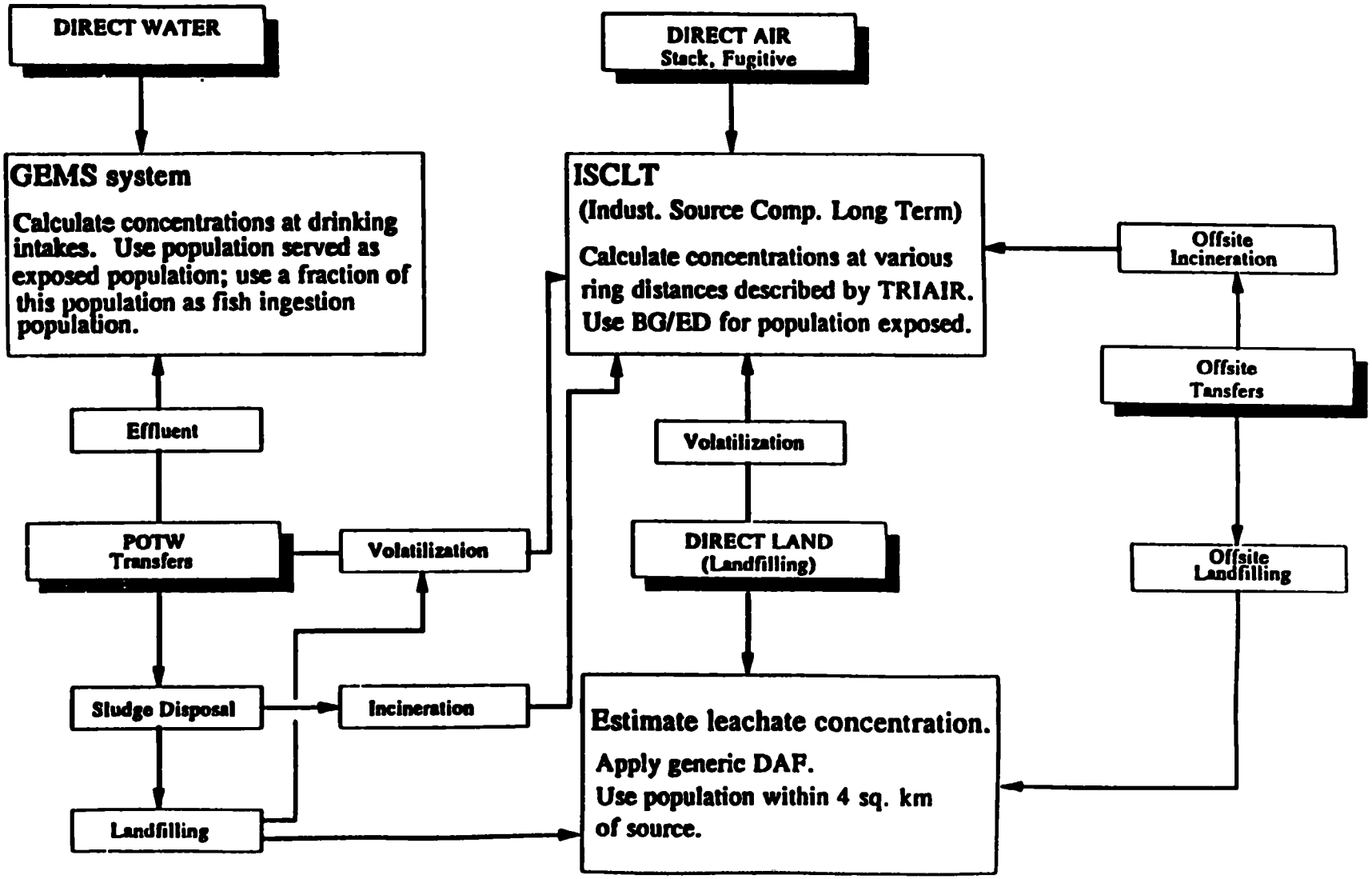
# FIGURE 9

## Overall Approach for Modeling TRI Discharges



from certain media may be evaluated in a more refined way than releases to other media. Furthermore, TRI release data are generally estimates rather than precise quantifications of releases, and, since we lack site-specific data, other modeling inputs would by necessity be generic. It may not be useful to perform modeling if release data are estimated and if inputs to the model are necessarily generic. All of these points argue for using a more simple approach to evaluating exposure.

However, even generic modeling has significant advantages. First, while modeling may not allow precise estimates of exposure due to generic and estimated inputs, it does allow us to estimate the magnitude of exposure and to consider local conditions where these data are available. In short, uncertainty should not be introduced where alternatives exist. Furthermore, to compare and sum exposure from different media, each media contribution must be expressed in an equivalent form, i.e., estimated "surrogate dose." In each pathway discussed below, surrogate dose can be estimated via generic modeling of each facility release and then can be coupled with toxicity to constitute a facility-chemical-media-specific increment to the entire indicator. No other method allows for this uniform element calculation. Without this common denominator, we would be forced to evaluate how a proxy measure of groundwater exposure (based on solubility) can be compared to a proxy measure of air exposure (based on photolysis rate). The relative ease of modeling releases to different media remains a problem; however, it may be appropriate to have better estimates of exposure for certain pathways if these pathways cause significant impacts and would contribute disproportionately to the indicators. For example, from a population perspective, it may be important to better understand air releases than offsite transfers since air releases will probably contribute far more to population impacts than transfers to hazardous waste facilities. In general, the Work Group preferred modeling where possible since it is the common Agency mechanism for incorporating emission data, local conditions, and population density into an exposure evaluation.

The exposure evaluation scheme presented below does not lend itself to quick calculation by hand, though hand calculation is not unimaginable. However, its structure offers unlimited combinations and views of the indicators' components. On one level, overall computation of the indicators could not be more replicable or verifiable, since it will be performed completely within one computer program. However, each facility-chemical-media indicator element could be disseminated in computer format for those wishing different views of its makeup. Regions, states, or individuals could use these individual constituents to create their own subindicators.

The following discussions of exposure frequently mention concentration and surrogate dose. We do not mean to imply that we somehow supplanted the risk assessment process and can accurately calculate cases. We speak of those terms only in the abstract. The method is a simple way to gauge relative risks from releases to different media in a congruent, defensible way. In some cases, the modeling will be purposely simple, given our lack of site-specific data. The differences in the level of refinement of exposure modeling are addressed by using the uncertainty weighting scheme discussed in Section IV.



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## Treatment of Emissions Range Reporting

Emissions data are a fundamental element of the exposure evaluation process. As discussed above, TRI facilities report emissions to seven pathways. Emissions data can be presented as numerical point estimates, or, if releases are below 1,000 pounds, as an estimated range of emissions. Where emissions are reported as a range, we could either use the midpoint of the range or the upper bound of the range to represent the emissions of that chemical. To produce a conservative estimate of exposure potential, we will use the upper bound of the range as our estimate of emissions, since this value is the maximum that the facility could be emitting.

## Stack and Fugitive Air Releases

Ideally, reported stack and fugitive air releases from the TRI database would be modeled using site-specific data (such as source area or stack height). Since TRI does not contain such facility-specific information, we must use default values to model TRI facilities with established EPA air dispersion models.

For this methodology, we will use the Industrial Source Complex Long Term (ISCLT) model developed by the Office of Air Quality Planning and Standards (OAQPS). ISCLT is a steady-state Gaussian plume model used to estimate long-term pollutant concentrations downwind of a source. The concentration is a function of site-specific parameters (stack height, stack velocity) and chemical specific decay rates.[3] The general form of the concentration equation from a point source at a distance $r$ greater than 1 meter away is[4]:

$$C_{air,jk} = \frac{2K}{\sqrt{2\pi}\, r\theta} \cdot \frac{Q f S V D}{u \sigma_z}$$

where

| | | |
|---|---|---|
| $C_{air}$ | = | concentration at distance $r$ ($\mu g/m^3$), |
| Q | = | pollutant emission rate (g/s), |
| f | = | frequency of occurrence of wind speed and direction, |

[3]Importantly, chemicals with extremely short half-lives in air will not be modelled using these procedures. Such chemicals will be assumed to degrade before significant exposure occurs. Products of decay could also be modeled where data permit.

[4] This equation is from EPA (1992). The equation is for a specific wind speed, direction, and category (*ijk*). Each facility has several combinations of these that must be added to arrive at a total concentration at that point. The equation for area sources is similar.

| | | |
|---|---|---|
| $\Theta$ | = | sector width (radians), |
| S | = | smoothing function used to smooth discontinuities at sector boundaries, |
| u | = | mean wind speed (m/sec), |
| $\sigma_z$ | = | standard deviation of vertical concentration distribution (m), |
| V | = | vertical term (m), |
| D | = | pollutant-specific decay in air ($e^{\text{distance} * \text{decay coefficient}/\text{wind speed}}$), and |
| K | = | scaling coefficient for unit agreement. |

For each facility in the TRI data set, a stack height of 10 meters will be assumed and ring radii from 50 meters to 50 kilometers from the source will be specified. For wind speed and direction, ISCLT can use Stability Array (STAR) weather data to measure typical wind speed and direction around a given source.

A variety of output is available from the model run, including concentrations at various distances from the source. The modeled concentrations at various distances can be combined with Block Groups/Enumeration Districts (BG/ED) data from the Census Bureau to arrive at population-weighted exposure values. The weighted concentration can be combined with standard assumptions regarding inhalation rate and human body weight to arrive at a surrogate dosage:

$$DOSE = \frac{C_{air,avg} \cdot I_{air}}{BW}$$

where

| | | |
|---|---|---|
| DOSE | = | surrogate dose of contaminant (mg/kg-day), |
| $C_{air,avg}$ | = | population-weighted average air concentration (mg/m$^3$), |
| $I_{air}$ | = | inhalation rate (m$^3$ per day), and |
| BW | = | human body weight (kg).[5] |

Figure 10 graphically describes the air modeling portion of the indicator, and Table 9 lists the default parameters for ISCLT.

Direct Surface Water Releases

The Graphical Exposure Modeling System (GEMS) contains capabilities for estimating concentrations in surface water from direct chemical discharges (EPA, 1987b). We will adopt GEMS data and methods for modeling surface water exposures. GEMS uses water volume data (from the GAGE database) and a routing database (the REACH database) that maps the path of the chemical to determine concentration. Another database

[5]This method uses the average adult body weight (male and female combined). for certain health endpoints (e.g., female reproductive effects), a different body weight value may be more appropriate (e.g., average adult female body weight).

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# Figure 10
## Stack and Fugitive Air Releases

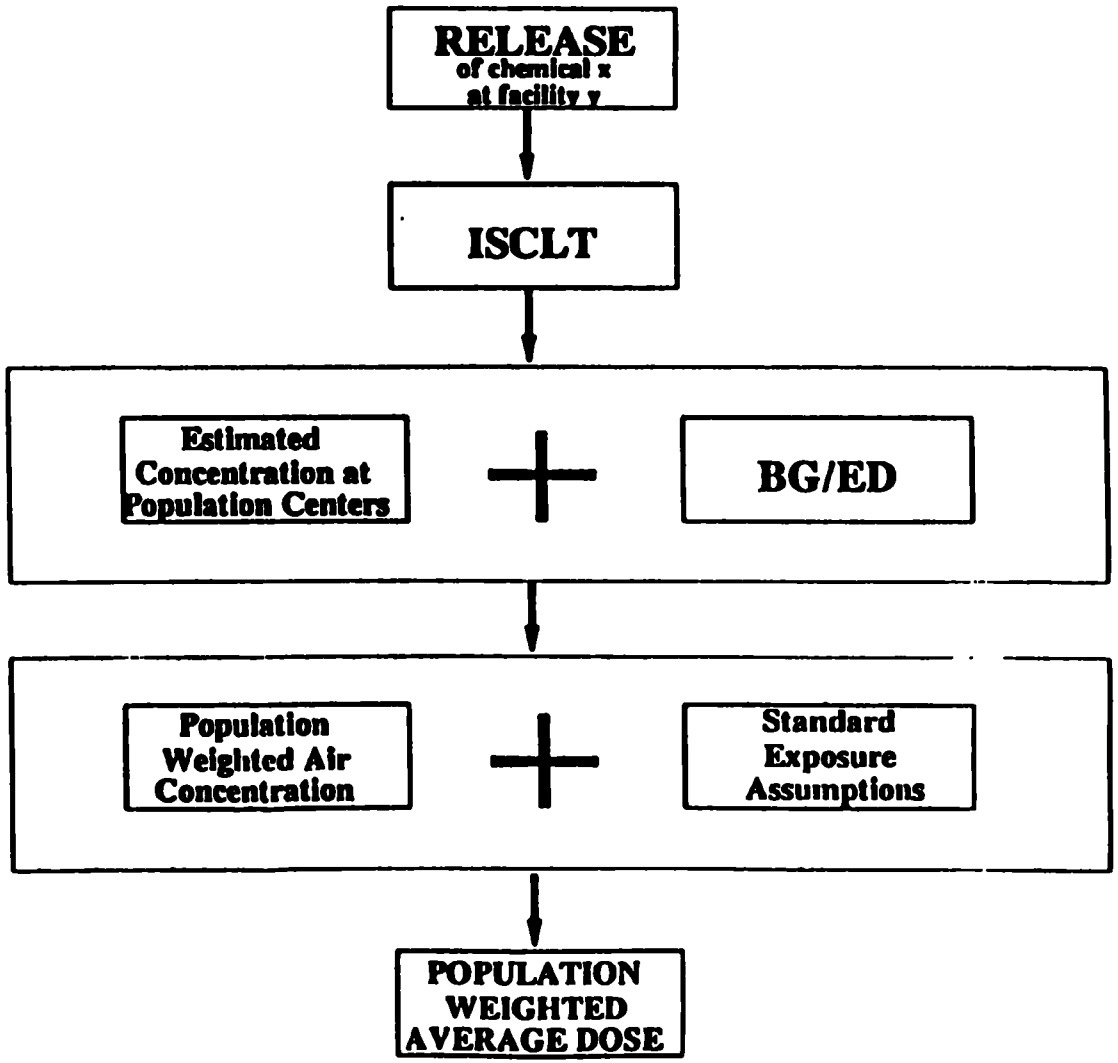

Table 9
Air Modeling Parameters

| Parameter | Value | Source/Comment |
|---|---|---|
| Stack height | 10 m | EPA (1992) |
| Exit velocity | 0.01 m/s | EPA (1992) |
| Stack diameter | 1 m | EPA (1992) |
| Exit gas temperature | 293° K | EPA (1992) |
| Area source size | 10 $m^2$ | EPA (1992) |
| Area source height | 3 m | EPA (1992) |
| Decay rate | varies by pollutant | |
| Body weight | 70 kg | EPA Exposure Factors Handbook (EPA, 1990a.); value is for adults; lifetime age-weighted average (male and female combined) is about 62 kg |
| Pollution emission rate | site-specific | TRIS (lbs/yr) |
| Freq. of wind speed and direction | site-specific | STAR |
| Sector width | 22.5° | 360° divided by 16 wind direct. |
| Wind speed | site-specific | STAR (m/s) |
| Smoothing function | calculated | |
| Vertical term | calculated | |
| Pop.-weighted average air conc. | calculated | mg/kg-day |
| Inhalation rate | 20 $m^3$/day | EPA Exposure Factors Handbook (EPA, 1990a.) |



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Federal Reporting Data System (FRDS) is accessed to determine the populations at drinking water intakes.[6]

GEMS uses a simple first-order decay equation along with volume and water speed estimates to calculate concentrations at a distance at time *t*. The general form is as follows[7]:

$$C_t = C_0 e^{-k_{water} t}$$

where

$C_t$ = concentration at time t,
$C_0$ = initial concentration, and
$k_{water}$ = decay coefficient.

Using the REACH database, which contains information on the stream network of the United States, discharges can be modeled as they make their way through the surface water network. Facilities can be matched to appropriate streams using the NPDES (National Pollutant Discharge Elimination System) numbers provided in TRI.

This methodology will consider two human health exposure pathways from surface water releases. First is the drinking water pathway. As the pollutant passes through the stream network, concentrations at public drinking water intakes can be noted and the population served can function as the exposed population at that concentration. The population-weighted water concentration is combined with standard exposure parameters to yield the following surrogate dosage:

$$DOSE = \frac{C_{water,\,avg} \cdot I_{water}}{BW}$$

where

DOSE = surrogate dose of contaminant (mg/kg-day),
$C_{water,avg}$ = population-weighted average water concentration (mg/l),

---

[6] This database has a limitation in that it generally captures only those public systems that serve populations greater than 2500. Locations for community systems serving smaller populations are sporadically available.

[7] Chemicals with extremely short half-lives in water will not be modelled using this procedure. Such chemicals will be assumed to degrade before significant exposure occurs.

$I_{water}$ = drinking water ingestion rate (l/day), and
BW = human body weight (kg).

As suggested by this equation, this methodology will not account for any removal of contaminants by drinking water treatment plants, nor does it account for the formation of contaminants during the chlorination process. The method also does not currently account for products of decay, although these could be included where data permit.

A second potential exposure pathway is from consumption of contaminated fish. For this pathway, fish concentration is estimated from water concentration:

$$C_{fish} = C_{water} \cdot BCF$$

where
$C_{fish}$ = concentration in fish, (mg/kg),
$C_{water}$ = average water concentration in stream (mg/l), and
BCF = bioconcentration factor for chemical (l/kg).

Next, the fish concentration value is combined with standard exposure assumptions regarding fish consumption rates to determine exposure from this pathway:

$$DOSE = \frac{C_{fish} \cdot I_{fish}}{BW}$$

where
DOSE = surrogate dose of contaminant (mg/kg-day),
$C_{fish}$ = fish tissue concentration (mg/kg),
$I_{fish}$ = fish ingestion rate (kg/day), and
BW = human body weight (kg).

We will use a fraction, yet to be determined, of the population served by drinking water intakes as an estimate for the number of persons that engage in recreational fishing in an area.

Figure 11 shows our recommended surface water approach, and Table 10 lists model parameters for surface water modeling.

<u>On-Site Land Releases</u>

On-site land releases include releases to landfills, surface impoundments, land treatment units and underground injection. This section describes methods to evaluate exposure from these releases. For simplicity, the following discussion will focus on landfill



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disposal, but the same evaluation principles will apply to the other types of land releases, with the exception of underground injection.

We are currently investigating methods to evaluate exposure from underground injection of TRI chemicals. Under well-managed conditions, these facilities are designed to pose minimal risks to human health or the environment. However, certain conditions can lead to the failure of these facilities and the release of chemicals to human and environmental exposure pathways. An exposure analysis for these releases would have to include an evaluation of the likelihood of the failure as well as an evaluation of the exposure impacts of such a failure.

Two major pathways are considered for on-site land releases: chemicals may volatilize to air or leach to groundwater. Volatilization of chemicals from on-site landfills is reported under the fugitive emission estimate for the facility and is thus handled as a direct air release.

Groundwater contamination is also a concern for land releases. However, the modeling of groundwater releases will depend on the regulatory status of the unit. Chemicals could be deposited in an on-site RCRA-regulated hazardous waste unit, or in an on-site nonhazardous solid waste management unit. RCRA standards for hazardous waste units are, by regulation, designed to include technical controls to prevent release of contaminants into groundwater; if chemicals are placed in such regulated units, it will be assumed that releases to groundwater are negligible. If chemicals are placed in RCRA nonhazardous land disposal units, we will model the release of chemicals to groundwater.

The TRI forms provide some clues regarding the regulatory status of land-disposed chemicals, but provide no site-specific information that aids in the evaluation of groundwater transport, such as geohydrological data. Unfortunately, these data are extremely site-specific and are not amenable to characterization by state or region of the country. In light of these limitations, we considered two possible approaches to evaluating groundwater contamination potential. First, we could simply use a measure of a chemical's mobility in groundwater (such as solubility and $k_{oc}$ value) in conjunction with the size of nearby populations as a proxy for exposure potential. The major drawback to this approach is that the exposure measure would be inconsistent with the exposure endpoint modeled for direct air and direct water releases (i.e., the meaning of the measures would not be comparable).

To maintain a concentration/exposure measure consistent with the approaches suggested for direct air and water releases, we propose an approach that gives a concentration at the exposure point (the well) to be combined with exposure assumptions to yield a surrogate dose. This approach requires two steps: estimating leachate concentration (a measure of the amount of chemical that partitions from the waste to water) and estimating the dilution and attenuation of leachate from the disposal site to the well location. The approach to evaluating exposure from landfilling is summarized in Figure 12.

# Figure 11
## Direct Water Discharges

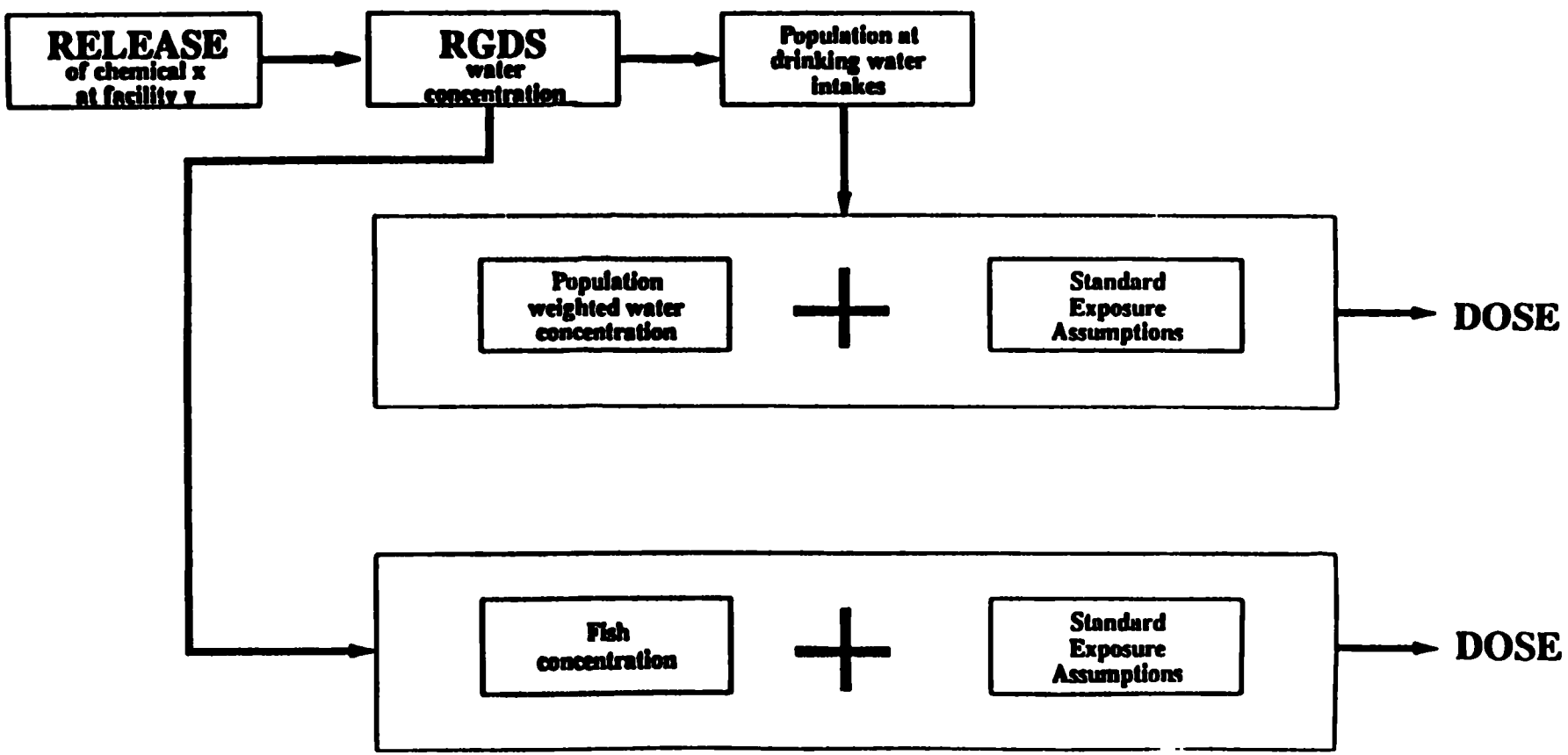

Table 10
Surface Water Modelling Parameters

| Parameter | Value | Source/Comment |
|---|---|---|
| Decay rate | varies by pollutant | |
| Dilution rate | site-specific | REACH (EPA, 1987b.) |
| Water volume and speed | site-specific | REACH (EPA, 1987b.) |
| Population-weighted average water conc. | calculated | mg/kg-day |
| Drinking water ingestion rate | 2 liters | EPA Exposure Factors Handbook (EPA, 1990a.) |
| Body weight | 70 kg | EPA Exposure Factors Handbook (EPA, 1990a.); value is for adults; lifetime age-weighted average (male and female combined) is about 62 kg |
| Average chemical concentration in stream | calculated | mg/l |
| Bioconcentration factor | varies by pollutant | l/kg |
| Fish tissue concentration | calculated | mg/kg |
| Fish ingestion rate | 0.0065 | kg/day; Exposure Factors Handbook (EPA, 1990a.) |

Leachate concentrations can be estimated using a modified modeling approach with chemical-specific parameters. The general form of this estimate is as follows:

$$C_l = \frac{C_s}{K_d \times B_d}$$

where

$C_l$ = concentration in leachate (kg/l or $1 \times 10^6$ mg/kg),
$C_s$ = concentration in landfill solids ($kg/m^3$ or 1000 mg/kg),
$K_d$ = soil/water partition coefficient (l/kg), and
$B_d$ = bulk density of material in landfill ($kg/m^3$).

This equation assumes that the landfill material essentially contains close to 100% solids. This assumption (and the equation) will have to be modified for use for surface impoundments. It must be noted that the concentration in the leachate, $C_l$, must be compatible with the chemical-specific solubility so that the smaller of the two values is used.

$C_s$, the concentration in the landfill solids, can be estimated by dividing the total mass of contaminant disposed (mg/yr) by the total mass of waste disposed in the unit each year:

$$C_s = \frac{M_c (mg\ per\ yr)}{M_w (kg\ per\ year)}$$

where:

$M_c$ = total mass loading of contaminant to landfill (mg per year), and
$M_w$ = total mass of waste disposed in landfill (kg per year).

The value for $M_c$ is available in the TRI database; the value for $M_w$ will be taken from EPA (1988b). This report summarizes the distribution (by number of facilities and by industry type) of the tons per year of waste disposed in industrial nonhazardous solid waste landfills. Data are also reported for surface impoundments, waste piles and land treatment facilities. These summaries are reproduced in Appendix E. It should be noted that using $M_w$ as the divisor in landfill concentration may underestimate the concentration of the TRI chemical, since the landfill may include some of the same chemicals from sources other than TRI facilities.

A summary of the values used in the groundwater calculation and the sources of these values appear in Table 11.

Once leachate concentrations are estimated, the next step is to determine the magnitude of dilution and attenuation of contaminants that occur as the contaminant travels from the source to the well. The Office of Solid Waste performed an analysis of dilution

and attenuation of contaminants in groundwater during the development of the Toxicity Characteristic Leaching Procedure (TCLP) rulemaking (55 (61) Federal Register 11798). For that rule, OSW used Monte Carlo analysis to evaluate dilution and attenuation factors (DAFs) for 44 chemicals. In the Monte Carlo analysis, multiple iterations of a groundwater model were performed. For each model run, model parameters values were drawn randomly from their distributions. (It should be noted that distance to the well was one of the parameters varied in the analysis: the distribution of distance between a source and a well was derived from a survey of Subtitle D facilities). The result of the analysis was a distribution of model results, where each model result was a DAF. OSW then selected the 85 percentile DAF for use in its regulatory calculations. For most chemicals modeled, the 85th percentile dilution and attenuation factor was approximately a factor of 100. For this methodology, we will use the OSW 85th percentile dilution and attenuation factor of 100 to estimate groundwater concentrations from land releases. It should be noted that OSW's DAFs are not intended to reflect the effect of pumping in drinking water wells on the concentration of chemicals in groundwater, and thus calculation of TRI surrogate dosages are oversimplified.

The final challenge in the groundwater puzzle is determining populations potentially exposed to the estimated groundwater concentration. The population of persons served by well water is available for each county from the National Well Water Association data files. From these data, we can derive a "well water drinker" population density for each county. We will then calculate the population of well water drinkers within 4 $km^2$ of the landfill site as our exposed population.

Releases To POTWs

In 1988, 570 million pounds of TRI chemicals were discharged to the country's Publicly Owned Treatment Works (POTWs) compared with 360 million pounds discharged directly to surface waters. Modeling exposure from TRI discharges to POTWs requires consideration of (1) overall removal efficiencies of POTWs and resulting effluent discharges from POTWs and (2) residuals management at POTWs. A summary of our proposed approach to modeling POTW emissions is found in Figure 13.

Modeling the exposures from POTW effluent is inexact due to the lack of National Pollution Discharge Elimination System (NPDES) numbers for the receiving POTW. Without the NPDES number, the location of the POTW facility can only be determined indirectly. Other OPPT efforts using TRI data have constructed approaches to locate POTWs. They involve name or zip code matches with databases to arrive at a NPDES number for the POTW and thus determine effluent streams and exposed drinking water populations. Ideally, a separate effort could be undertaken to match POTWs in TRI with NPDES numbers. Such a match would greatly enhance modeling POTWs. Absent such an effort, we will use the POTW zip code as its geographical locator.

# Figure 12
## Direct Land Releases

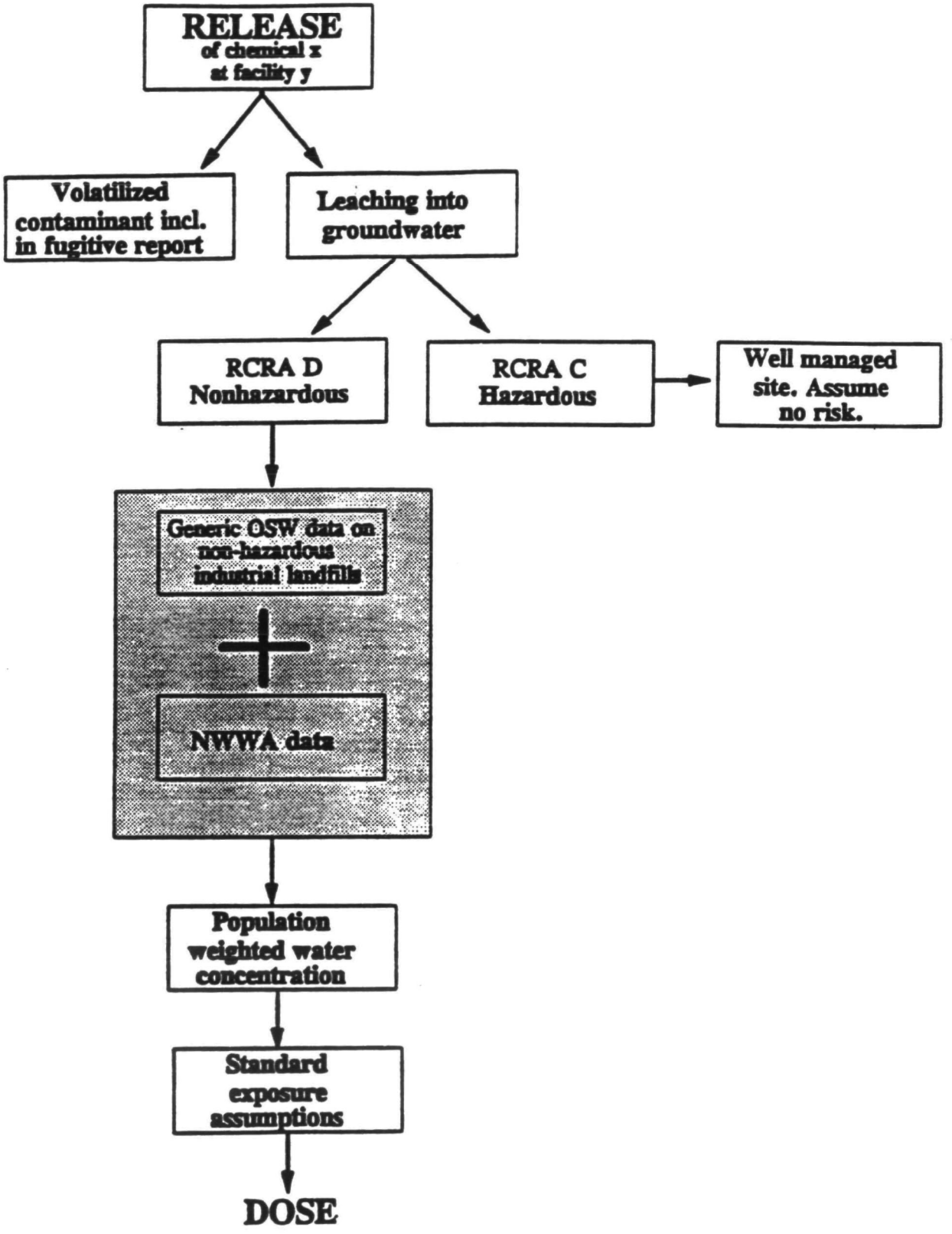

Table 11
Groundwater Modelling Parameters

| Parameter | Value | Source/Comment |
|---|---|---|
| Concentration in landfill waste | calculated | calculated from TRIS data and from industry-specific mass of waste disposal per year (see Appendix E) |
| Concentration in leachate | calculated | mg/l |
| Bulk density | 400 $kg/m^3$ | calculated from data in EPA (1988b) |
| Partition coefficient | varies by pollutant | |



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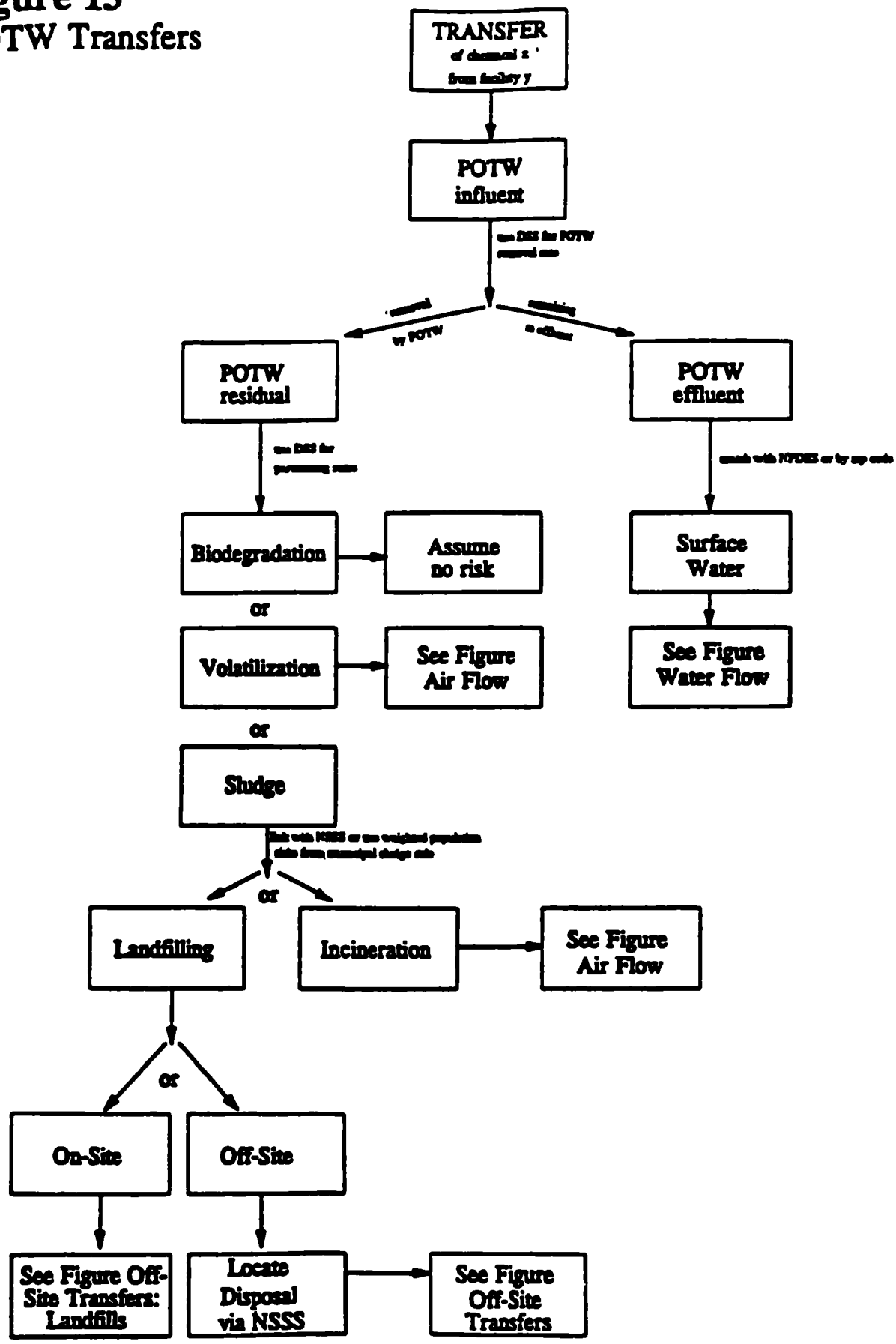
# Figure 13
## POTW Transfers



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POTWs are not completely effective at removing all of the chemicals in the influent; some of the chemical loading in the influent will be released in the POTW effluent. Typical overall POTW removal efficiencies vary by chemical. Chemical loadings that are removed by POTW treatment processes partition to several pathways within the POTW, including biodegradation, volatilization, and adsorption to sludge. Using average removal and partitioning rates, chemicals will be divided among effluent, biodegradation, air and sludge pathways. The Domestic Sewage Study (EPA 1986c) gives both typical POTW removal efficiencies and within-POTW partitioning rates for many TRI chemicals. These values will be used in this methodology. Chemicals lacking partitioning rates will be assigned rates based on their chemical class. To do so, each chemical having partitioning rates in the Domestic Sewage Study will be assigned to a class (halo-organic, metal, etc.), and an average determined for each class. The average rate will be applied to other TRI chemicals in that class lacking specific partitioning rates.

Once the fates of chemicals entering the POTW are determined, the exposure levels associated with chemical loadings to each compartment will be estimated. Chemicals that escape in the POTW effluent will be modeled using the surface water evaluation methods described above. Chemicals that biodegrade will be assumed to cause no further exposure. POTW volatilization releases will be treated like area-source air releases, as described above.

For chemicals that partition to sludge, the models used to depict exposure will depend on the sludge disposal method employed by the POTW. The remaining problem is to determine which POTWs engage in which sludge disposal practices. A database does exist (the National Sewage Sludge Survey) that describes the sludge disposal methods employed by POTWs in the United States. The exposure levels from POTW sludge contaminants can be modeled using the same methods used to model direct releases of contaminants, depending on the POTW sludge disposal practice (incineration, landfilling, land application, etc.). If extracting data on disposal practices is too cumbersome or if a match cannot be found, other methods for modeling these exposures will have to be adopted. One possible method is to use results from the national aggregate population risk assessment for municipal sludge performed in support of upcoming municipal sludge rules. From this risk assessment, we could obtain average exposures per ton of sludge disposed, by disposal method. These results could be used for this analysis by weighting these unit exposures by the amount of sludge disposed by each practice (either regionally or nationally), then multiplying by the tons of sludge disposed by the POTW (which can be estimated based on flow to the POTW).

Off-Site Transfers

In 1988, over 17 percent of TRI volume was transferred to off-site locations for storage or disposal. Figure 14 presents a summary of our proposed method to model off-site transfers. TRI reporters are supposed to supply the name and address of the receiving facility. From these data, we must determine if wastes are sent to a hazardous or

nonhazardous waste management facility. Efforts are currently underway between OSW and OPPT to match facilities reported in TRI with RCRIS reporting to aid in making this determination. Chemical submissions indicating transfer to a RCRA hazardous waste facility will not be included in the indicator; for the purposes of simplifying the indicator calculation, these transfers are assumed to pose no further risk in a regulated disposal facility.

For some off-site facilities, the TRI form will report the treatment or disposal method employed. Chemicals sent to facilities where the treatment method is unknown will be assigned among treatment technologies, based on the distribution of methods practiced at Treatment, Storage or Disposal Facilities (TSDFs) where the treatment/disposal method is known.

The exposure evaluation for off-site transfers will obviously depend on the type of treatment/disposal employed off-site. We are still investigating methods for evaluating exposures from various treatment and disposal technologies, including underground injection. We currently have methods to evaluate exposure from two offsite disposal technologies: waste incineration and landfilling.

Air releases from off-site waste incinerators can be modeled like direct air releases. We will obtain removal efficiencies for nonhazardous waste incinerators from an OSW analysis of municipal solid waste combustion (EPA, 1987a).

For landfills, two major pathways will be considered. The groundwater pathway will be modeled for off-site releases in the same manner as for on-site land releases. Volatilization, however, will be handled differently. For on-site releases, volatilization is included in reported fugitive emissions and thus exposure is modeled with air releases. For off-site land releases, volatilization emissions from land disposal must be estimated before exposure can be modeled. Since the volatilization rate is a function of vapor concentration, the vapor concentration must be calculated. This involves two steps: partitioning from the solid to the water, and then water to air. Simple steady-state relationships can be used to approximate these partitioning processes if certain chemical-specific data are known.

The equation for determining the concentration of chemical in the liquid phase (i.e., leachate) was given earlier in the "On-Site Land Release" section:



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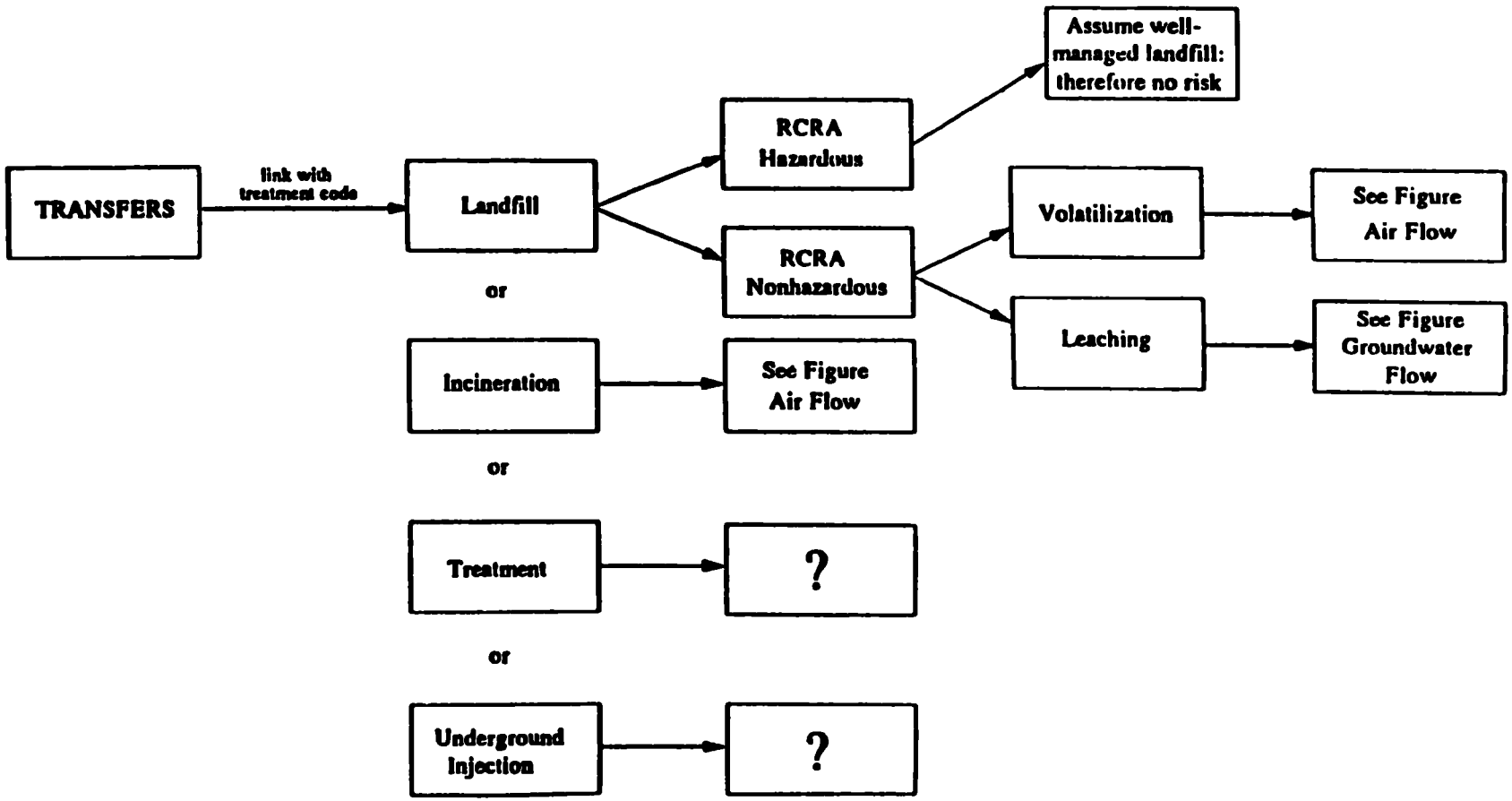
# Figure 14
## Off-Site Transfers



$$C_l = \frac{C_s}{K_d \times B_d}$$

where

$C_l$ = concentration in leachate (liquid phase) (kg/l),
$C_s$ = concentration in landfill solids (kg/m$^3$),
$K_d$ = soil/water partition coefficient (l/kg), and
$B_d$ = bulk density of material in landfill (kg/m$^3$).

The second calculation determines the vapor phase concentration from the liquid phase concentration using Henry's Law Constant (the ratio of the contaminant concentration in the vapor to the concentration in the liquid phase):

$$C_v = H\, C_l$$

where

$C_v$ = concentration in vapor phase (kg/l) and
$H$ = Henry's Law Constant (dimensionless).

Now that an equilibrium vapor concentration has been determined, the rate of volatilization may be estimated from a first-order rate equation:

$$Vol\ Rate = k_{vol}\, C_v$$

where

$k_{vol}$ = volatilization rate constant.

The volatilization rate constant is taken from a EPA (1985) equation for uncovered monofills:

$$k_{vol} = \frac{0.17\, u\, (0.994)^{(T - 20)}}{\sqrt{MW}}$$

where

$u$ = wind speed (m/s),
$T$ = ambient air temperature, assumed to be 15°C,
MW = molecular weight (g/mol) and
0.17 and 0.944 are empirical constants.

All of these formulae may be combined to express the volatilization rate as a function of the chemical concentration in the solid phase:



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$$Vol\ Rate = \frac{0.17\ u\ (0.994)^{(T-20)}\ H\ C_s}{k_d\ B_d\ \sqrt{MW}}$$

These volatilization emissions estimates, along with weather and population data, will be used to arrive at population-weighted concentrations in the same way as fugitive direct air releases from TRI facilities. Population will be extracted using the zip code of the receiving facility. Volatilization parameters are summarized in Table 12.

## VI. COMPUTATION OF THE INDICATORS

This section of the report summarizes the actual computation of the TRI indicators and the adjustments made to the indicators when chemicals or facilities are added to theoriginal set of TRI chemicals and facilities. The methods of calculating the indicators are presented first; subsequent discussion focuses on methods to accommodate additions of both chemicals and facilities to the indicators.

Before describing its calculation, we will reiterate a few characteristics of the TRI indicators. First, two chronic indicators will be calculated, one to measure the impacts imposed on human health and the other to measure impacts on the environment. Dividing the indicators into categories allows us to examine fluctuations in each category. Second, the actual indicator quantity yields a general measure of related to risk but does not translate into a physically meaningful term, e.g., the statistical risk to an individual. Third, two chronic indicators (i.e., human health and ecological) with the same score do not necessarily share the same absolute risk. Again, it is the relative change to the previous score that make the TRI indicators useful instruments.

Fourth, it is important to remember that the TRI indicators are rough measures only of the impacts of the TRI chemical releases, a subset of the total universe of chemicals being released into the environment. The indicators gauge neither the impacts of chemicals regulated in other programs within the EPA nor the impacts of chemicals that lie wholly outside of EPA regulation. In the future, the indicator scores will represent the impacts of additional chemicals and facilities yet to be added to the program; however, the initial indicator scores will reflect only the impacts of the current roster of TRI chemicals, facilities, and media.

When chemicals and facilities are added to the TRI roster in the future, the numerical value of the indicators would almost certainly increase if no adjustments were made to the method of calculation to account for the additions. However, such an increase would not necessarily represent a sudden increase in actual environmental impact, but rather would reflect a broader understanding of the impacts that had existed all along. To maintain comparability in the indicators' scores over time, the indicators would have to be

Table 12
Volatilization Modelling Parameters

| Parameter | Value | Source/Comment |
|---|---|---|
| $K_d$ | varies | Chemical properties database |
| Molecular weight | varies | Chemical properties database |
| Henry's Law Constants | varies | Chemical properties database |
| Average area of source: municipal solid waste landfill | 32.5 | in acres; from EPA (1988c) |
| Median area of source: industrial nonhazardous land disposal | landfill: 3<br>surf.impndmt: 0.5<br>land trtment: 15<br>waste pile: 0.5 | in acres; from EPA (1988d) |
| Mean wind speed | site-specific | m/s; from STAR data |



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adjusted in some manner when such additions occur. We address this issue in the following sections.

Indicators Computation

The indicators will be calculated by combining the individual TRI chemical-facility-media indicator elements. As discussed earlier, each element's value is a measure of a chemical's impact on either human health or the environment (depending on the indicator) based on some measure of the volume of release from a facility, the chemical's toxicity, and the potential exposed population for the media of release. We propose two alternative ways of calculating the indicators:

Simple Sum of the Component Scores:

$$I = S_1 + S_2 + S_3 + \ldots + S_n$$

where

I = TRI indicator of interest and
S = facility-chemical-medium-specific indicator element.

In this method, each component score makes a contribution proportional to its size. Simply, it is the total impact resulting from all chemical-facility-media releases. The final value would be scaled to a manageable number for ease of presentation to the public. For example, in the first year, the final number could be scaled to 10,000, and subsequent year numbers would be scaled so that they could be compared to 10,000.

Simple Sum Normalized to a Base Year:

$$I = \frac{(S_1 + S_2 + S_3 + \ldots + S_n)_{present\ year}}{(S_1 + S_2 + S_3 + \ldots + S_n)_{base\ year}} \cdot 100\%$$

Like the simple sum method, this method represents each component score proportionately. Its primary advantage is that it is a dimensionless ratio that tracks progress over time and continuously looks back at the beginning of the indicator record. With a score of 100 in the base year, a score of 60 in year 2 and 40 in year 3, the indicator value has been reduced by 40 percent in year 2 compared to the base year, 60 percent in year 3 compared to the base year, and 20 percent from year 2 to year 3. Thus, the score would reflect change from year to year, and from the base year. It must be reiterated that while such a trend in scores over the years would imply that there has been a decrease in environmental effects, the magnitude of the decrease is unknown.

Other Methods of Calculation Considered

Alternative means of calculating the indicators were considered. Some of these included the arithmetic mean of the component scores, the geometric mean of the scores, and the least-square difference of the scores. Each of these methods generates a score that will fluctuate as the individual components of the indicator fluctuate. However, the methods do not produce readily interpretable results, and detecting fluctuations is less obvious than with more straightforward methods. For the greatest degree of variability in the actual indicator score, as well as for the greatest ease in calculation and interpretation, we recommend that the chemical-facility-media elements simply be added and then adjusted to a manageable level.

Normalizing the Indicators

An increase in the number of components of the TRI can occur through any of three mechanisms: an addition of chemicals to the TRI list, an increase in the number of facilities by enhancing the SIC code list, and an increase in facility compliance with existing reporting requirements. Each of these scenarios enhances the accuracy of the report because they supply missing information. However, this addition changes the scope of the indicators (from a small subset to a larger subset), thereby limiting the effectiveness of comparison between current and past values.

The addition to or deletion of chemicals from the TRI roster will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. The deletion of chemicals will presumably have a minor effect since such chemicals would be deleted due to their low risk; by definition these chemicals will make only a minimal contribution to the indicators. Deletion will most likely occur in batches every few years. The addition of SIC codes will likely follow investigations of the TRI chemicals revealing other industries that emit the listed chemicals. Compliance with TRI reporting could also improve in the future. In 1989, the Office of Toxic Substances studied compliance with TRI reporting requirements. The study found that the compliance rate was 81.7 percent in the first year of reporting. Follow-up studies have not been done to determine the improvement in compliance with Section 313. However, the OPPT study stated that under full compliance, the estimated number of respondents would be over 29,000. In the last two years of reporting, the number of reporting facilities has not approached that figure, despite a lowering of reporting thresholds.

The fundamental problem we face when chemicals or facilities are added to or deleted from the TRI roster is that there is no way to differentiate between indicator fluctuations due to changes in environmental impacts and those due to changes in the chemical roster. Therefore, if the indicators are to be compared year to year, then each addition to the indicators must be accompanied by some kind of adjustment to the indicator calculation so that the integrity of the indicators is preserved. The Work Group considered several methods for accommodating the addition of chemical-facility-media elements,



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including: (a) the creation of separate indicators for new chemicals and facilities, (b) a ratio adjustment method, and (c) the initiation of new indicators upon addition of many new chemicals and facilities (the "starting over" option). Details of each of these methods, and their advantages and disadvantages, are found in Appendix F. The Work Group identified two of these options as the most feasible and easily interpretable.

The first option is to create new indicators when significant new additions are made to the TRI roster. "Significant" additions could be several minor additions that have been made over the course of a few years that eventually add up to a significant change, or a single major influx of new chemicals (due to Congressional action, for example). These new indicators would include both old and new chemicals and facilities, but would provide a mechanism to track the initial set of chemicals and facilities so that trends could be discerned for that subset.

A second option is to simply start over when significant new additions are made, without subsequent tracking of subsets. This approach would also allow modifications to the calculation methods that may be desired based on experience with the indicators from previous years. This second option would be accompanied by a thorough explanation to the public regarding why the initial set of indicators are being abandoned and a new set of indicators adopted.

## VII. ABIOTIC INDICATORS

The Work Group considered expanding the set of TRI indicators to include indirect health and environmental impacts from TRI releases. Examples include deposition of airborne chemicals into other media, such as surface water; global climate change; acid deposition; ozone depletion; and tropospheric ozone formation (smog formation).

Since each of these indirect effects are effects on human health and the environment, it would seem necessary to include them in a set of indicators which measures environmental impacts from TRI releases. However, the complexity of and uncertainty in modeling these scenarios makes direct insertion into our current indicator algorithm extremely difficult. The following discussions examines indirect health and environmental impacts, their potential inclusion into the TRI Environmental Indicators, the potential creation of separate indicators, and the difficulties in accomplishing either.

### Global Warming

Some of the TRI chemicals are considered "greenhouse gases." These chemicals, when released into the atmosphere, can absorb infra-red radiation which the earth emits as it establishes radiative equilibrium with the solar system. The potential result of this "effect" is the increase of the average temperature of the earth's surface, an increase which could lead to higher sea levels, droughts, floods, and climate changes.

The quantification of these risks is a hotly contested topic in academic, political and industrial circles. The potential temperature increases have been predicted to be anywhere between zero and eight degrees Celsius. The direction of the climate change resulting from the accumulation of greenhouse gases can be offset by natural occurrences such as volcanic eruptions or the appearance of El Niño, a circulating body of abnormally warm water in the Pacific Ocean. Since the results of the buildup of greenhouse gases have not been, and quite possibly cannot be, quantified, it is impossible to assign a greenhouse effect risk to the unit emission of a greenhouse gas. Thus the greenhouse effect cannot effectively be incorporated into the TRI Environmental Indicators.

This is not to say that the release of greenhouse gases, and their relative threat, cannot be traced with a separate indicator. In attempting to quantify the climate change potential associated with gaseous emissions, greenhouse gases have been weighted relative to their capacity to absorb infra-red radiation and their half-life in the atmosphere. These weights have been normalized to $CO_2$, the greenhouse gas greatest in both presence in the atmosphere and rate of addition to the atmosphere. The other major greenhouse gases are listed below:

| Trace Gas | Life (Years) | Global Warming Potential (Integration Time Horizon) | | |
|---|---|---|---|---|
| | | 20 yrs. | 100 yrs. | 500 yrs. |
| Carbon Dioxide | (120) | 1 | 1 | 1 |
| Methane | 10 | 63 | 21 | 9 |
| Nitrous Oxide | 150 | 270 | 290 | 190 |
| CFC-11* | 60 | 4500 | 3500 | 1500 |
| CFC-12* | 130 | 7100 | 7300 | 4500 |
| HCFC-22 | 15 | 4100 | 1500 | 510 |
| CFC-113* | 90 | 4500 | 4200 | 2100 |
| $CCl_4$* | 50 | 1900 | 1300 | 460 |
| $CH_3CCl_3$ | 6 | 350 | 100 | 34 |
| $CF_3Br$ | 110 | 5800 | 5800 | 3200 |
| CO | <1 | 7 | 3 | 2 |

* - TRI Chemical

Source: EPA (1990b)

The emissions of greenhouse gases can be reported by their relative weight of contribution to the greenhouse effect and reported in a simple indicator. For CFC-11, -12, -13 and carbon tetrachloride, the indicator developed here for global warming potential would be an additional measure of these chemicals' environmental hazard. That is, each of the chemicals listed above will also have human health and ecological effects captured by the



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TRI Environmental Indicators method described in earlier sections. The global warming indicator would supplement the set of TRI Environmental Indicators to provide an overall measure of these four chemicals' potential to cause environmental damage.

We should note that the TRI data base is quite limited in its ability to assess overall global warming potential from air releases of U.S. point sources. In fact, only four of the eleven chemicals that are key contributors to global warming are currently reported in TRI. Thus, any separate attempt to measure trends in global warming using the TRI database should consider these limitations.

Acid Rain

Acid rain results from the deposition of sulfur- and nitrogen- containing compounds, particularly sulfur dioxide and nitrous oxides, into clouds. The sulfur and nitrogen react with the water to form sulfuric and nitric acid which then accompany water during precipitation, leading to corrosion of structures and reductions in the pH of soils and water. Some researchers have attributed the elimination of habitat in different parts of the world to acid rain, particularly in areas where coal provides the primary energy source for combustion processes.

Like the greenhouse effect, it is extremely difficult to determine the effect caused by the unit emission of an "acid rain" chemical. The amount of sulfur and nitrogen which may combine to form an acid depends upon equilibrium concentrations in the area of concern. Although the acidity of sulfuric acid and nitric acid may be compared directly by their respective pH at a given concentration, and although the number of sulfur or nitrogen atoms present in a compound may determine the ability of a chemical to contribute to the creation of these acids, site-specific conditions will determine the quantity and concentration of the acids.

Like the risks associated with global warming, the risks posed to human health and the environment from acid rain have not been quantified in terms of individual toxic risks. Some work has been done on health conditions and respiratory problems. However, most work concerning acid rain has focused on population-based economic risks, a different perspective than the one used to determine the TRI Environmental Indicators. The health effects seem to have been precursors to determining factors such as days lost at work and other economic inputs.

Furthermore, $SO_x$ and $NO_y$, the primary substances linked to the formation of acid deposition particles, are not currently included in the TRI list of chemicals for which reporting is required. In addition, coal burning power plants are not included among SIC codes 20-39. As such, those facilities who are among major emitters of acid deposition precursors are also not required to report under TRI. If in future rulemaking under SARA Section 313 these substances and sources are added to the TRI list, then an indicator could be developed to track progress in reducing acid deposition.

Stratospheric Ozone Depletion

The depletion of the stratospheric ozone layer results from the reaction of chlorine and fluorine atoms in chlorofluorocarbons with ozone, breaking the ozone down into diatomic oxygen and oxygenated compounds. Since ozone absorbs incoming ultraviolet radiation, the deterioration of the ozone layer is resulting in dramatic increases in environmental exposure to UV radiation. This high-energy end of the spectrum has been shown to cause cataracts, suppress the immune system and induce cancer in humans. It has also been shown to adversely affect plant and animal life. Thus, the risks to humans could lie anywhere from actual health hazards to loss of agriculture.

A major project at EPA focused on determining the risks associated with CFCs and their alternatives in order to formulate policy options. The model tracks emissions into the atmosphere, models the reduction in the ozone layer, and calculates risks and damage associated with skin cancer, cataracts, aquatic impacts, crop loss, immunosuppression, and even a qualitative assessment to the food chain (starting with oceanic plankton). The model is complicated but could be used to determine risks associated with the emissions of CFCs.

A weighting scheme has been developed to determine the effectiveness of different CFCs at depleting the ozone layer. These weights are detailed below:

| Substance | Domestic 1986 Use (millions kg) | Weight | Weighted Production |
|---|---|---|---|
| CFC-11* | 91.3 | 1 | 91.3 |
| CFC-12* | 146.2 | 1 | 146.2 |
| CFC-113* | 71.1 | 0.8 | 56.9 |
| CFC-114* | 4.1 | 1 | 4.1 |
| CFC-115* | 4.61 | 0.6 | 2.8 |

* - TRI Chemicals: Chlorinated Fluorocarbons are a category in the TRI.

Source: Hahn and McGartland (1989)

A separate indicator could be developed for ozone depletion through the use of these weights. The indicator would serve as an approximate measure of these group of chemicals contribution to stratospheric ozone depletion. This measure obviously would not be complete since some chemicals (e.g., HCFCs) and many sources (e.g., home and car air conditioning systems) are not included in the current TRI reporting requirements. Nevertheless, a number of stratospheric ozone depleting chemicals and some production and use sources are included in TRI, so that TRI and this indicator could provide some general trends in tracking releases of these substances.



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For the individual substances listed above, this stratospheric ozone depletion indicator would provide an additional measure of these chemicals' relative environmental hazard. For example, a carcinogenic substance such as carbon tetrachloride will be captured by the human health and environmental indicators described in earlier sections. Carbon tetrachloride would also be included in the stratospheric ozone depletion indicator as well as the global warming indicator. Thus, the stratospheric ozone depletion indicator will provide a supplemental measure of environmental damage of each of the chemicals listed above.

Tropospheric Ozone

The creation of tropospheric (low atmosphere) ozone, one of the main constituents of the lower atmosphere, results from the reaction of a radical oxygen atom with an oxygen molecule. This maverick oxygen atom is produced when ultraviolet radiation in sunlight breaks apart a nitrogen dioxide atom into nitrous oxide and oxygen. In normal circumstances, the ozone will react with the nitrous oxide in order to reform the nitrogen dioxide and the diatomic oxygen, the preferred state. However, the presence of volatile organic compounds (VOCs) in the air prevent this elimination of ozone by reacting with the nitrous oxide, creating nitrogen dioxide before the molecule can react with ozone. Thus it is the presence of both $NO_x$ and VOCs that lead to the formation of ozone in the troposphere.

The presence of ozone in the troposphere poses human health and environmental risks since it is this level of the atmosphere in which we live. Ozone causes respiratory ailments, particularly in the older and younger populations, and is an eye irritant.

The difficulty with pinning down the effects of emissions of either nitrous oxides or VOCs is their dependence upon one another for the creation and destruction of ozone. Rural and urban areas will have different impacts from increased or decreased emissions of VOCs.

Reporting of VOCs as a group and $NO_x$ are currently not required by TRI. VOCs could be derived by identifying all individual organic chemical compounds currently reported in TRI that are considered tropospheric ozone precursors. An indicator could then be derived by summing all those compounds for each facility. An alternative approach would be to simply add by rulemaking VOCs and $NO_x$ as a group. In this way, analyzing these substances and developing the indicator for tropospheric ozone precursors from TRI facilities would be straightforward. A third approach would be to not develop a TRI indicator at all for VOCs since the Clean Air Act requirements necessitate monitoring and reporting of emissions of these substances in ozone non-attainment areas.

Particle Deposition

Particle deposition differs from the volatilization pathway currently analyzed in the TRI Environmental Indicators by tracing airborne emissions through exposure scenarios other than inhalation. Particles can land on clouds and precipitate, entering water bodies and exposing populations through drinking water. Particle deposition can also produce risks to both humans and wildlife through direct ingestion of soils and dust and by consuming food crops grown on agricultural land.

Many models have been developed at ORD to determine the exposure posed by particle deposition. We are investigating these methods for their potential incorporation into the indicators method.

## VIII. PROPOSED COMPUTER ALGORITHM FOR CALCULATING THE TRI INDICATORS

Preceding sections discussed the general methodology for calculating the TRI Environmental Indicators. Each component part was addressed and its calculation or use was outlined. As presented in Section VI, the indicators are designed as the sum of constituent facility-media-chemical "elements":

$$I = S_1 + S_2 + S_3 + \ldots + S_n$$

where

I = TRI indicator and
$S_n$ = facility-chemical-medium-specific element.

After the program runs, as many as 500,000 indicator elements will be summed to yield just one of the raw TRI indicators (e.g., the Human Health Chronic Indicator). How do we arrive at the half million elements to begin with? This section addresses the automated approach to calculating the elements. The computer algorithm used to calculate the TRI Environmental Indicators can be thought of as a three-part process; input, exposure modeling, and element calculation. This section describes each of these parts. First, we describe the fundamental data input files common to all of the element calculations. Next, we provide a step-by-step description of how these data files are linked with mathematical models and the exposure and toxicity weighting matrices in order to calculate the elements. The step-by-step description also delineates the format and content of additional data files that are specific to the analysis of particular release pathways. A summary of the step-by-step process is provided in Appendix G.

Before we begin to construct an algorithm for indicator calculation, we must first select a programming language in which to implement the algorithm. We propose to use the Statistical Analysis System (SAS). SAS is a data management and analysis programming language widely used in government and industry. In fact, an outstanding TRI analysis

system, TRIPQUIC, uses SAS code to provide a rich set of exploratory tools. Its flexibility and power are unsurpassed among major data management systems. The choice to use SAS allows greater control of the input and output sequences and easily allow virtually limitless views of an indicator's make-up.

General Data Input

To support the calculation of the indicators, we will create or use a variety of data files.[7] The program will then access these data files to obtain model input parameters as the models are run. Because the TRI database is continually updated and so fluctuates over time, we will use data from the two week period each year when EPA freezes the database for analysis. All of the TRI Environmental Indicators calculations rely on three major data input files. First, the RELEASE[8] file contains information on releases for each facility-chemical combination in the TRI data base. The RELEASE file contains values for releases to all media and is the core of the indicators calculation. In the input process, data will be checked for errors and, if possible, corrected.[9] Variables essential to indicator calculation that are contained in the file are listed below.

| Variable | Comment | Variable | Comment |
|---|---|---|---|
| TRI_ID | Unique facility identifier | ACTFLAG | Activity/use flags |
| DCN | Identification number used for matching facility with data in other data files | FUGAIR | Fugitive air emission of chemical from the facility (pounds per year) |
| ZIPCODE | ZIP code of the facility | STKAIR | Stack air emission of chemical from the facility (pounds per year) |
| NPDES | NPDES permit number of the facility | WATER | Direct water discharge emission from facility (pounds per year) |
| LATITUDE | Latitude for facility | LAND | On-site land release from facility (pounds per year) |

[7]We refer to data files by a capitalized one word file name. This is only for clarity in the discussion; the actual locations and names of files appear in footnotes.

[8] Text file - TRIS.PROD.CHEMICAL.FILE89. This file was created to assist in creating the TRI National report. The entire file format is available from EPA.

[9] The exact details of how various errors will be treated will be discussed in the final report.

| | | | |
|---|---|---|---|
| LONGITUDE | Longitude for facility | UI | Release from facility to underground injection (pounds per year) |
| SIC | SIC code of facility | POTW | Discharge of chemical from facility to POTW (pounds per year) |
| CAS | CAS number of chemical | TRANSFER | Transfer of chemical off-site from facility (pounds per year) (other than POTW discharges) |
| TRIRCRA | RCRA ID number of TRI facility (if it has one) | BASIS1-BASIS5 | Basis/method for estimating the quantity of release (separate variable for each type of release) |

The ACTFLAG variable indicates how the chemical is used at the TRI facility. Although this variable has no direct role in indicator calculation, it will be useful for performing diagnostics on the indicators. Similarly, the method for estimating the quantity of the release is included as the variable BASIS and can be used for performing diagnostics on the indicators.

The second fundamental input file is the BGREACH file, which contains information on the populations and geographies of areas surrounding TRI facilities.[10] The BGREACH file was inspired by the current efforts to develop a GIS (Geographic Information System) at EPA. The file is a two-dimensional digital representation of the United States. As seen in Figure 15, the country is divided into 1 kilometer square cells.[11] For each of these cells, a variety of geographical information about the location can be stored. Storing information in this manner allows us to access all of the relevant geographical information for each TRI facility by simply accessing the BGREACH cell that matches the location of the facility. This approach has significant advantages over having to access a number of different data files to retrieve different pieces of geographical information. Although the BGREACH file is not an exact reproduction of the geography and demographics of the U.S., it is a reasonably good approximation for our purposes. The variables contained in the BGREACH file are listed below.

[10] FBXTRIS.TRIDENT.BGREACH - This file is a SAS housed on the EPA mainframe developed for this project.

[11] The choice of 1 kilometer is somewhat arbitrary. The size of each square can be set to any value. However, halving each squares area quadruples the size of the file.



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| Variable | Comment | Variable | Comment |
|---|---|---|---|
| CELLXY | Cartesian location of the cell | FLOW | Water volume (million liters per day) |
| POP | Population in the cell | WATERPOP | Population at intake |
| NEARSTAR | Nearest Weather Station ID | FIPS | State-County FIPS Code |
| WELL | Well density in cell | NEXTXY | Next cell for stream |

Other variables can be added to the file if necessary. To build the BGREACH file, we will need to extract data from a variety of sources. Enumerated below are explanations of each variable, sources used to obtain data on the variable, and the weaknesses of each variable.

1. CELLXY - This value describes the relative location of the cell on the grid. This variable is the basic identifier that will be used to link the information in BGREACH file with information from the RELEASE file and other data files. We will link BGREACH to the RELEASE data by using the latitude and longitude data of the TRI facilities. To link the location of a TRI facility to a CELLXY value, the equivalent cartesian (x and y) distances of the TRI facility latitude and longitude are first calculated from a central point in the continental United States (96 degrees longitude and 37 degrees latitude). After these distances are calculated, a cell address can be directly calculated as follows:

$$Cell_{xy} = (y+1600)\cdot 10^4 + (x+1600)$$

where

$Cell_{xy}$ = cell address or location file,
y = north/south distance (km) to center of US, and
x = east/west distance (km) to center of US.

Adding 1600 (km) to the x and y distances guarantees positive values.

2. POP - This variable represents the number of people living in the cell. Information on populations will be extracted from the Census Bureau's BG/ED file. The BG/ED file reports population and longitude/latitude pairs for centroids of Block Groups and Enumeration Districts.[12] Each centroid will be converted into a cell address ($Cell_{xy}$) based on the above equation. Populations with equivalent cell

[12] Block Groups and Enumeration Districts are terms used by the Census Bureau to describe very small units or blocks within metropolitan areas and rural areas generally containing not more than 800 people.

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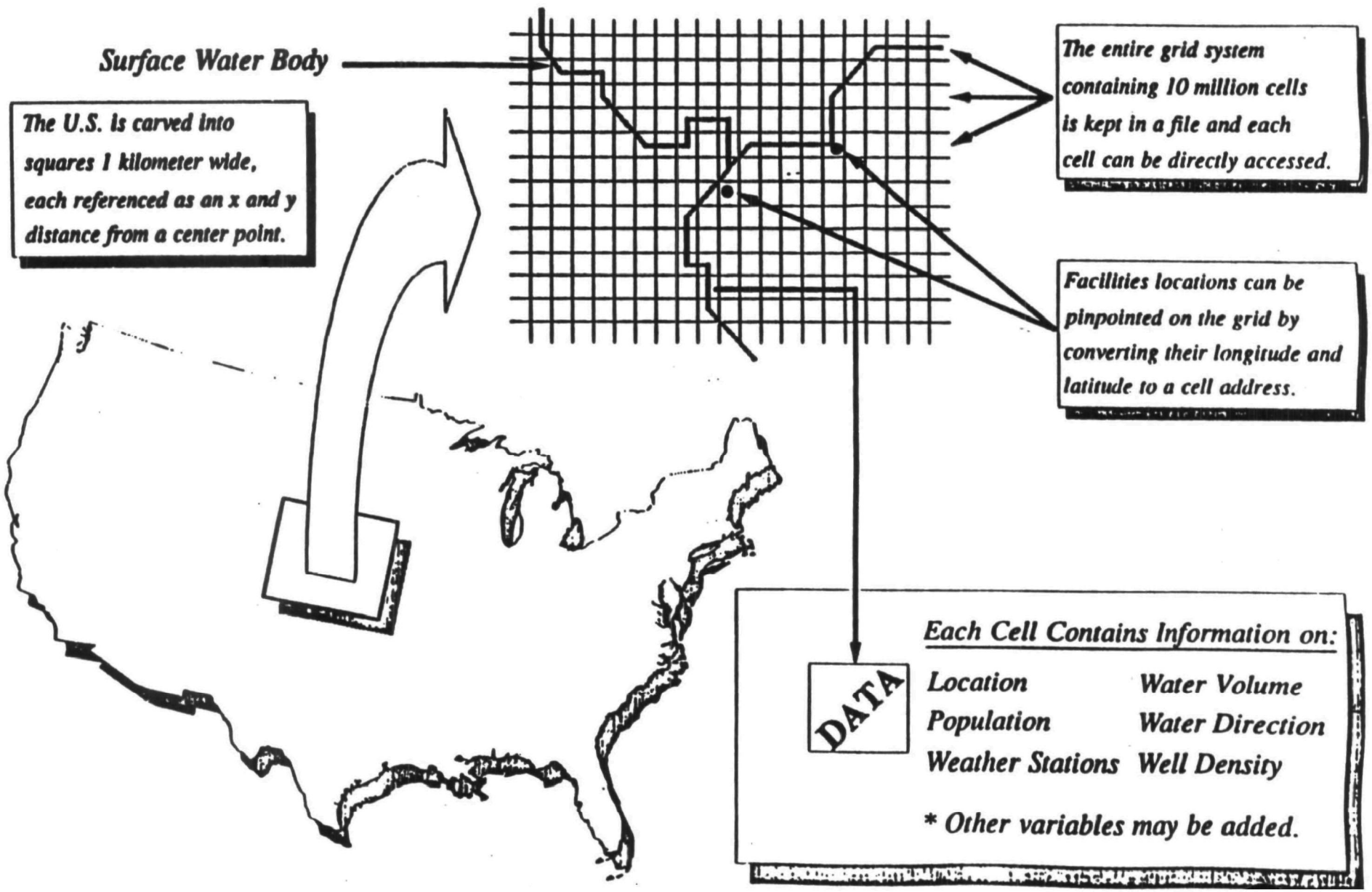
# Figure 15
## How the TRI Indicator Program Views the United States



addresses will be summed. This exercise yields a population number for each inhabited square kilometer in the United States.

One problem in this approach is that the land area of rural districts can be larger than a square kilometer. These areas are treated the same as a city block. In other words, a cell in the BGREACH file may contain a population that is actually spread over several kilometers. One way to adjust for this is to assume a uniform population distribution and allot populations to surrounding cells based on the reported size of the Enumeration District. However, since we propose in our methodology to set populations to a minimum value of 1,000, and since the population in an Enumeration District is usually less than 1,000, uniformly distributing populations is not necessary.

3. NEARSTAR - This variable identifies the location of nearby weather stations. It contains an identification value for the nearest weather station from the STAR (STability ARray) database. Using this identification number, the most probable prevailing weather conditions can quickly be fetched from a companion weather data file.

4. WELL - Variable WELL is a percentage of cell occupants who receive their drinking water from groundwater sources. It comes from a National Well Water Association (NWWA) county level file with counts of persons and homes either having private wells or receiving water from a utility that uses groundwater as its source. The NWWA file is catalogued using state and county FIPS codes. To insert these data into our BGREACH file, we will first match the FIPS codes to the Census BG/ED data. We can then match the BG/ED data to the cell identifier (CELLXY) as described above.

5. FLOW - This variable contains the flow volume of the surface water body in the cell. We can get data on the continental stream network from the REACH file which is part of the Routing and Graphical Display System (RGDS). The stream network will be mapped onto the BGREACH grid system based on longitude and latitude coordinates of stream segments in the REACH file. Since segment lengths are often larger than our 1 km grid network, care will be taken to assure consecutive segments align within our grid. Essentially, the path of a surface water body will be tracked at 1 km intervals instead of the multiple mile intervals in REACH. This will not increase precision, however, since each grid cell that is part of a stream segment will contain the flow properties of the segment itself in million liters per day.

6. WATERPOP - This variable contains the size of the population served by a drinking water utility that has an intake within the cell's boundaries. Using this variable, we will be able to estimate the population exposed to chemicals in surface water in that cell. Data on the population served by drinking water utilities will be derived from FRDS.

7. NEXTXY - This variable contains the address of the cell into which the surface water body flows next. It is the link that allows us to follow the movement of chemical discharges through the surface water network.

The final fundamental input data file is the TOX file. This file contains chemical-specific toxicological and chemical properties data. These data will be linked via the chemical's CAS number to the RELEASE file and other data files.[13] The variables contained in the TOX file are listed below.

| Variable | Comment | Variable | Comment |
|---|---|---|---|
| CAS | CAS number | AQNOAEL | Life cycle or chronic No Observable Adverse Effect Level for aquatic life |
| WOE | EPA cancer WOE category | LOGKOW | Log of the octanol water partition coefficient |
| TSCAWOE | TSCA Chemical Scoring System cancer WOE category | SOL | Water solubility (mg/l) |
| QSTAR | Cancer potency estimate (kg-day/mg) WOE | AIRDECAY | Decay rate in air ($hr^{-1}$) |
| ED10 | Effective dose, 10 percent (dose lethal to 10% of test animals) (mg/kg-day) | WATERDECAY | Decay rate in water ($hr^{-1}$) |
| RFD | Reference dose (mg/kg-day) | KOC | Soil-water partition coefficient |
| WOENC | EPA noncancer WOE category | POTWREMOVE | POTW removal efficiency |
| TSCAWOENC | TSCA Chemical Scoring System noncancer WOE category | POTWVOL | Percent of chemical that volatilizes at the POTW |

[13] FBXTRIS.TRIDENT.TOX.PHYSCHEM - SAS file housed on the EPA mainframe. This file will also be available in dBase III and Lotus 1-2-3.

| | | | |
|---|---|---|---|
| LOAEL | Lowest Observable Adverse Effect Level (mg/kg-day) | POTWSLUDGE | Percent of chemical that partitions to sludge |
| NOAEL | No Observable Adverse Effect Level (mg/kg-day) | POTWDEG | Percent of chemical that degrades in the POTW |
| MED | Minimum effective dose (mg/kg-day) | DRE | Removal efficiency for municipal waste incinerator |
| LC50 | Lethal concentration, 50 percent (concentration lethal to 50% of test organisms | HC | Henry's Law constant |
| AAWQC | Acute Ambient Water Quality criteria or Ambient Aquatic Life Advisory Concentration | MW | Molecular weight |
| CAWQC | Chronic Ambient Water Quality Criteria or Ambient Aquatic Life Advisory Concentration | BCF | Bioconcentration factor |

Sections IV and V of this report describe the meaning and the sources of information for each of these variables.. In addition, Appendix C presents the values for some of these variables for many of the TRI chemicals.

## Modeling Process

In Section IV, weighting schemes for toxicity and exposure evaluations were described. In Section V, the mathematics behind modeling exposure were discussed. In this section, we simply outline the mechanics of combining the data files described above with (a) the mathematical equations that predict exposure and (b) with the weighting schemes used to derive the toxicity and exposure potential weights. The final facility-chemical-medium-specific element is the product of the toxicity weight, exposure weight and estimated population size.

1. Air Releases - A facility directly releasing to air is first located on the BGREACH grid. The data in the BGREACH file are used as inputs to the ISCLT model equations discussed in Section V. At each of the 100 cells (10 km x 10 km) nearest to the facility, the program calculates a concentration based on the ISCLT equations. To perform these calculations, weather data (not included in BGREACH) are needed. The weather data are stored in the STAR[14] data file. Variables included in the STAR dataset are given below.

| Variable | Comment | Variable | Comment |
|---|---|---|---|
| ID | STAR Station ID | MEANWIND | Mean wind speed |
| LONGITUDE | Longitude of the station | CATEGORY | Stability category |
| LATITUDE | Latitude of the station | F1-F16 | 16 frequencies of occurrence |

The NEARSTAR variable in the BGREACH file is matched with the ID variable in the STAR data file.

The concentration calculated in each cell is then weighted by the population in the cell to derive a population-weighted average concentration over all 100 cells. If a cell contains no population, a value of 10 is used in the cell to assure that the population surrounding a facility is at least 1000 (i.e., there will be 100 cells with at least 10 persons in each cell).

Once the population-weighted concentration is estimated, the program derives the surrogate dose using the surrogate dose calculations described in Section V. The program then uses the exposure weighting matrix (presented in Section IV) to assign an exposure weight to the calculated surrogate dose. For the air release pathway, we propose to use uncertainty category A to classify the air exposure potential (see Section IV discussion of exposure potential uncertainty).

Finally, the program accesses the TOX data file to assign a toxicity weight. The toxicity weighting matrix used by the program is presented in Section IV. The product of the exposure score, the toxicity score and the size of the population over the 100 cells yields an indicator element for the facility-chemical-air release combination. We propose to use uncertainty category A for the air pathway, since the population exposed via this route is fairly well characterized (compared to other pathways).

[14] FBXTRIS.TRIDENT.STAR - SAS file containing weather information used in air modelling. The file was converted to SAS for this project. It contains the same data used by ISCLT.

2. Water Releases - A facility discharging to water is located on the BGREACH grid and, using the water volume data contained in the BGREACH file, an initial concentration is calculated at the cell containing the facility. Then, based on the NEXTXY variable in the BGREACH file, the surface water body is traversed and the concentration is adjusted along the water body.

Two exposure pathways are calculated from these water concentrations. First, exposures from drinking water are calculated. If a cell contains no drinking water intake, the WATERPOP variable is zero; otherwise, the WATERPOP variable is non-zero. The concentrations in the cells with a drinking water intake are converted to surrogate doses using the surrogate dose equations described in Section IV. The calculated surrogate doses are weighted by the population in the cell to derive a population-weighted average surrogate dose. As with the air releases, the program then uses the exposure weighting matrix to assign an exposure weight to the calculated population-weighted surrogate dose. For the drinking water pathway, we propose to use uncertainty category B for exposure potential weighting for several reasons. First, the calculation of water concentrations does not consider partitioning of chemical between the water column and suspended solids, deposition of the sediments along the water course, or other processes that may affect the fate and transport of contaminants along a surface water body. Furthermore, there is no consideration of the removal of contaminants during treatment of drinking water at the utility.

Finally, the program accesses the TOX data file to assign a toxicity weight based on the toxicity matrix presented in Section IV. The product of the exposure score, the toxicity score and the population for all of the cells with drinking water intakes yields a facility-chemical-drinking water element. For population uncertainty weighting, we propose to use category B; although we know the locations and populations served by drinking water with reasonable accuracy for systems serving more than 10,000 persons, we have only sporadic data about smaller systems.

Another possible exposure pathway for water discharges is the consumption of contaminated fish. Each segment of the affected water body may contain contaminated fish which could be caught and eaten by recreational fishers. As described above, the program will track the concentration of the chemical as it traverses down the waterway; at each cell, the concentration in fish will be derived and the resulting surrogate dose calculated using the surrogate dose equations presented in Section V. The calculated surrogate dose in each cell will then be weighted by the population of recreational fishers assumed to reside in that cell. This yields a population-weighted average surrogate dose for all cells. We will estimate the number of recreational fishers as the total population in the cell times a fraction of persons who are assumed to fish for recreation. The U.S. Fish and Wildlife Service produces a survey of hunting, fishing and wildlife every five years. The survey includes state-specific data on fishing rates that we could use to derive



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a state-specific fraction of persons who fish. As with the drinking water pathway releases, the program then uses the exposure matrix to assign a weight to the calculated population-weighted surrogate dose. For this exposure pathway, we propose to use uncertainty category C for exposure potential for several reasons. First, as with the drinking water pathway, the estimated water concentrations are probably an overestimate because we don't consider all processes in surface water that affect concentrations. Second, fish concentrations are actually dependent on the type of species, particularly its lipid content and its position in the food chain. Finally, the actual probability of recreational fishing in the particular stream reach being modeled is unknown, as is the actual quantity of fish consumed from that particular reach.

Next, the program accesses the TOX data file to assign a toxicity weight based on the toxicity weighting matrix presented in Section IV. The product of the exposure score, the toxicity score and the population for all of the cells traversed by the contaminated surface water yields an element for the facility-chemical-fish ingestion combination. For fish ingestion, we propose to use population uncertainty category C, since the actual number of persons fishing in the particular stream reach is a very rough estimate using generic data.

3. On-site Land Releases - Land releases, as discussed in Section V, can contaminate groundwater or can volatilize to air. For on-site land releases, the volatilization component should be reported under fugitive emissions and thus will be handled under the air release calculations. For groundwater releases, the exposure modeling will depend on the regulatory status of the on-site unit into which the chemical is released. Therefore, before any groundwater modeling can be conducted, the regulatory status of the unit must be determined. There are a number of ways to approach this problem. First, an effort could be undertaken to match the on-site land releases reported in TRI to the RCRIS database. This would allow us to obtain information on the type of units maintained by the TRI facility. Such a match could be achieved through the use of the unique RCRA ID number which is reported in both TRI (if the facility has such a number) and in RCRIS. However, such an undertaking may prove to be quite burdensome. A simpler approach would be to assume that if the TRI form reports a RCRA ID number for the facility, then the on-site land releases are assumed to go to a RCRA regulated unit. Otherwise, the on-site land release is assumed to occur in a nonhazardous land disposal facility.

If the release occurs in a nonhazardous unit, groundwater releases are modeled. As described in Section V, there are two steps to this process: modeling the leachate concentrations and then applying a dilution and attenuation factor to estimate the concentrations at the well. Since deriving leachate concentration is a function of the contaminant level in the waste, we must first estimate this value. The equation presented in Section V for calculating waste concentration requires an estimate of the waste volume generated by the industry on a yearly basis. The release loading



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can then be assumed to be dispersed throughout this waste volume. Appendix E contains the estimated waste volumes by industry. This appendix will be converted to a data file WASTE[15], with the following content:

| Variable | Comment | Variable | Comment |
|---|---|---|---|
| SIC | SIC code for which the waste volume is applicable | UNITTYPE | Type of management unit into which waste is placed |
| WASTEVOL | Industry-specific waste volume disposed per year | | |

Once the waste concentration is estimated, the program will access the TOX data file to obtain the partition coefficient necessary to calculate the leachate concentration, as described in Section V. The DAF (dilution and attenuation factor) of 100 then is applied to estimate the contaminant concentration at the well. The program uses the well concentrations to calculate an estimated surrogate dose, as described in Section V.

The program then uses the exposure matrix to assign a weight to the calculated surrogate dose. For the groundwater pathway, we propose to use uncertainty category C, since the exposure estimate is based on a conservative, steady-state estimate of leachate concentration, and on a conservative, generic dilution and attenuation factor.

The program then accesses the TOX data file to assign a weight based on the toxicity matrix presented in Section IV. The proposed population exposed to contaminated groundwater is calculated from the number of persons receiving drinking water from groundwater within 4 square kilometers of the facility. This value is included in the BGREACH file as the WELL variable. We propose to use population uncertainty category C for this pathway, since we do not know the areal extent of the potential groundwater contamination, the direction of groundwater flow, and other factors that would help us to estimate the number of persons drinking groundwater potentially affected by the facility.

The product of the exposure score, the toxicity score and the population over 4 $km^2$ yields an element for the facility-chemical-groundwater combination.

4. Releases to POTWs - Some facilities report discharges to POTWs. For these TRI releases, the modeling of the exposure potential requires information about the

[15]FBXTRIS.TRIDENT.WASTE - SAS file containing waste volume information.

location and certain characteristics of the POTW to which the TRI facility releases contaminants. To store POTW-specific information, we will use a data file called POTW.[16] The appropriate POTW file will be matched to the TRI transfer via the DCN (Document Control Number) variable in the RELEASE data file. Variables contained in the POTW file are shown below.

| Variable | Comment | Variable | Comment |
|---|---|---|---|
| DCN | ID used for matching with TRI transferring facility | ZIPCODE | ZIP code of the POTW facility |
| BASIS6 | Basis/Method for estimate of quantity of release to POTW | SLUDGE | Sludge disposal method employed by the POTW |

The ZIP code of the POTW is provided on the TRI form of the facility making the transfer. Using this data file, POTWs will be located on the BGREACH grid based on the latitude and longitude of the ZIP code centroid. To do so, we must match the ZIP code centroid with a latitude and longitude. This information will be stored in a data file called ZIPCODE.[17] The format of the ZIPCODE file is given below.

| Variable | Comment | Variable | Comment |
|---|---|---|---|
| ZIPCODE | ZIP code | FIPS | State-County FIPS CODE |
| LONGITUDE | Longitude of the ZIP code centroid | LATITUDE | Latitude of the ZIP code centroid |
| POP | ZIP code population | | |

Once we have located the POTW, the next step is to apply the overall POTW contaminant removal rate (stored in the TOX file) to the release. This overall removal rate allows the program to calculate the loading of contaminant remaining in the POTW effluent and the loading that remains in the POTW. Contaminants remaining in the POTW are partitioned within the POTW, using partitioning rates stored in the TOX file. The partitioning rates allow us to estimate the amount of contaminant in the POTW sludge and in the POTW volatile emissions, as well as the amount that degrades.

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[16] TRIS.PROD.POTW.FILE89 - This file is also part of the national report family of files. The full record layout is available from EPA.

[17] FBXTRIS.TRIDENT.ZIPCODE.CENTROID - SAS file containing FIPS, zipcode, longitude/latitude, and census information for all ZIP codes in the United States.

Once the program has accounted for the fate of all of TRI releases to the POTW, it models the exposure associated with each fate endpoint. First, the POTW effluent is modeled as a direct water discharge from the POTW. Since ZIP code centroids are used to locate the POTW, it is possible that a POTW may be placed on a BGREACH grid cell without a water body running through it. In this case, the water body receiving the POTW effluent is determined by finding the nearest water body to the ZIP code centroid. We could improve this estimate if we could find longitude and latitude information for POTWs from a source other than ZIP codes. Volatilization from POTWs is modeled as a fugitive emission. The method for modeling fugitive emissions is described in the Air Releases section above.

The sludge disposal practice employed by a particular POTW is not known from the TRI database. We will attempt to use the NSSS to identify sludge disposal methods for particular POTWs. If we are successful, we can then model the particular sludge disposal method using exposure evaluation methods described above. For incinerated sludge, destruction and removal efficiencies from the TOX file are applied and then air modeling is performed, as described in the Air Releases section above. Land disposal of sludge can be modeled as a land release using methods described above.

If the NSSS database cannot be employed to identify POTW sludge disposal practices, the impacts of sludge disposal will be quantified using chemical-specific weighted average unit exposure estimate derived from the national municipal sewage sludge aggregate risk assessment.

The resulting sum of the uncertainty-adjusted, population-weighted surrogate doses from POTW effluent, volatilization at the POTW, incineration of sludge, volatilization of land disposed sludge, and groundwater contamination from land-disposed sludge are combined with the chemical-specific toxicity score to yield a facility-chemical-POTW release element.

5. Transfers Off-Site - Some facilities report transfers to off-site facilities. As with POTW transfers, to assess exposure potential associated with off-site transfers, we must have information on the off-site facility location and some of its characteristics. To store off-site facility information, we will construct the data file OFFSITE.[18] Variables necessary from the file are shown below.

[18] TRIS.PROD.OFFSITE.FILE89 - This file is also part of the national report family of files. The full record layout is available from EPA.



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| Variable | Comment | Variable | Comment |
|---|---|---|---|
| DCN | ID used for matching TRI facility | RCRA-ID | RCRA ID number (if it has one) |
| ZIPCODE | ZIP code of off-site facility | BASIS7 | Basis/Method for estimating quantity of chemical transferred off-site |
| TREAT | Type of treatment | | |

We can match data in the RELEASE file to this file via the DCN (Document Control Number) variable. The ZIP code for the off-site facility to which chemicals are transferred is contained in the TRI data base. The ZIP code will serve, in conjunction with the ZIPCODE data file, to locate our facility on the BGREACH grid, as was described for locating POTWs. It should be noted that OSW and OPPT are jointly working on a tracking system to match TRI releases to the RCRIS data base. If this effort is completed before we implement the TRI Environmental Indicator, we may be able to use the fruits of that effort for more precise tracking of the off-site releases. Once we have located the off-site facility, we also need to know (a) the regulatory status of the unit to which the material is transferred and (b) the treatment/disposal technologies used by the off-site facility. The regulatory status of the off-site units could be determined in a number of ways. The TRI form requires the reporting facility to give the RCRA-ID number of the off-site facility to which the chemical is being transferred. We could assume that if such a number is reported, then the chemical is being transferred to a RCRA-regulated unit. Otherwise, we will assume that it is a RCRA Subtitle D nonhazardous management unit.

The TRI forms also require the reporting facility to indicate the treatment/disposal method used at the off-site facility. Where this information is reported, it is stored as the TREAT variable in the OFFSITE data file; the method reported will be assumed to be the treatment/disposal method employed by the off-site facility. If this information is not reported (despite the requirement), we will have to assume a distribution of treatment/disposal methods, based on the frequency of treatment/disposal methods reported for that chemical. Using this distribution, we will assign the appropriate proportion of the release to each reported treatment/disposal method.

Once the treatment method is established, we can model exposure potential using the methods described above. Incinerators will be modeled by applying destruction and removal efficiencies from the TOX data file and running the air model described in the Air Release section. Landfilling is treated the same as on-site land releases. Other treatment methods employed at off-site facilities (storage, underground injection) are being explored for possible incorporation into the indicators.

The resulting sum of the uncertainty-adjusted, population-weighted surrogate doses from incineration, volatilization and groundwater exposures are combined with the chemical-specific toxicity score to yield a facility-chemical-off-site release element.

Indicators Summation Process

After the elements are calculated, all the elements can be combined in limitless ways. Figure 16 shows how flexible this approach can be in tracking indicator differentials over time. Elements will be kept in a file each year so comparisons can be quickly made with previous years. The elements can also be combined and evaluated in other ways than annual comparisons. The detailed calculations used to create elements allow computation of "subindicators" for individual chemicals, geographic regions, industry sectors, facilities, or exposure pathways. These subindicators, like the overall indicator, cannot be compared to some absolute level of concern, but could help identify the relative contribution to various components to the overall estimate of emission impacts.

## IX. ISSUES FOR FUTURE CONSIDERATION

There are two general types of issues yet to be resolved: specific methodological questions for the indicators developed to date, and development of additional indicators. The methodological questions associated with the indicators developed to date that still need to be resolved include the following:

- How to address additions/deletions to the TRI chemical list, and whether to create new indicators when significant changes are made;
- How to include deposition of TRI chemicals into underground injection wells in the indicators;
- For noncarcinogenic chemicals without RfDs, what specific WOE systems should be used for neurotoxicity, reproductive toxicity, and other chronic toxicity endpoints;
- For offsite transfers, how to better match TRI transfers to particular treatment practices (e.g., which TRI chemicals are sent to hazardous or nonhazardous waste management facilities; use of specific treatment practices at POTWs; and how to estimate the potential impact of non-landfill, non-incineration treatment types); and
- Using initial results of indicator computations, an examination of the impact of various exposure weights and their WOE modifiers.

The possible development of indicators for acute human health effects and acute aquatic effects depends on improved toxicity and other data. In addition, as discussed in

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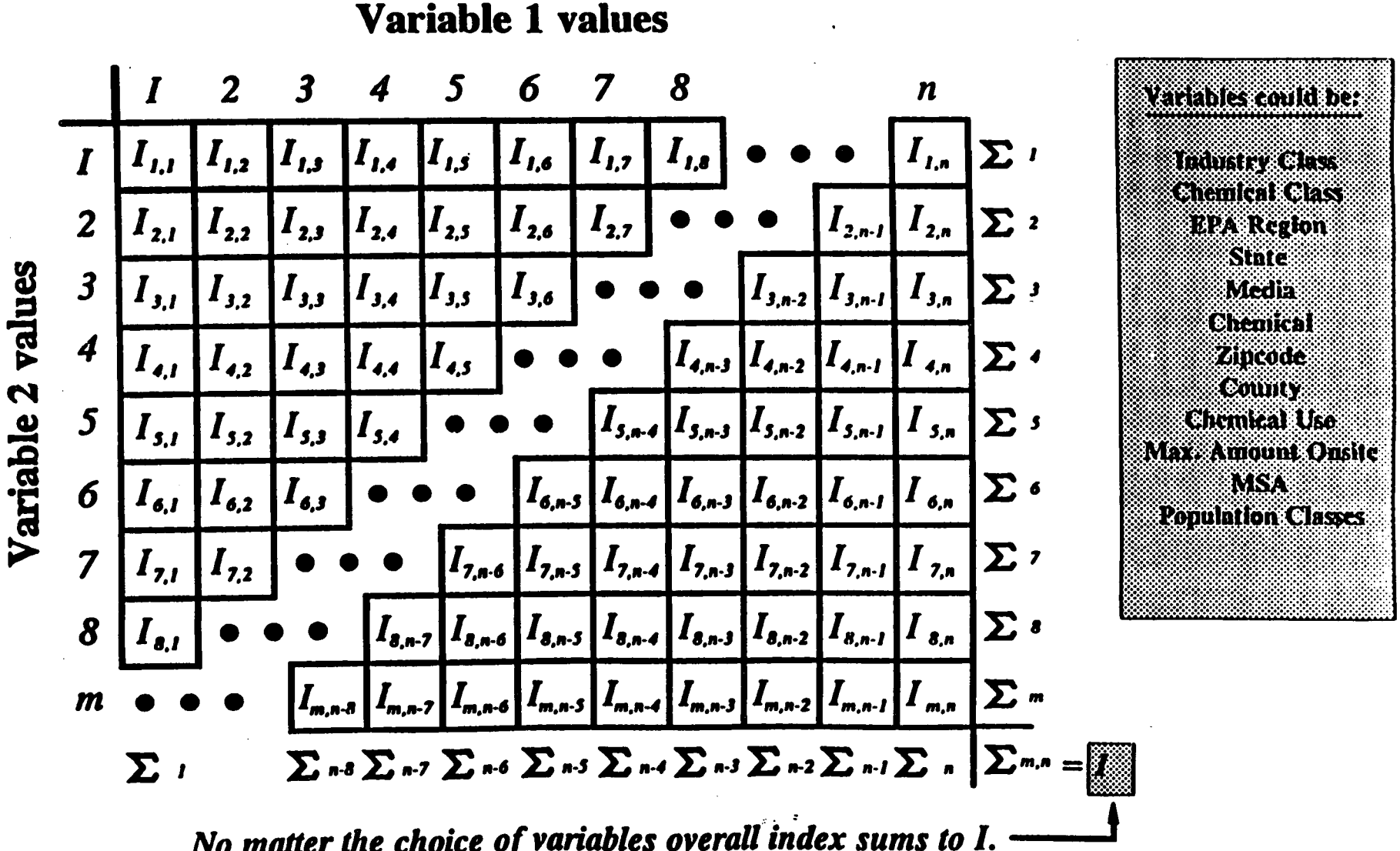
# Figure 16

## Reporting Subindices with TRI Index Component Method
## Calculating Facility-Chemical-Media Increments Yields Unlimited Flexibility



Section VII, EPA considered expanding the TRI Environmental Indicators to reflect indirect health and environmental impacts from TRI chemicals, such as global climate change, acid deposition, stratospheric ozone depletion, tropospheric ozone formation, and particulate deposition. While many of these impacts have health-related effects, the complexity and uncertainty in modeling them may make it impossible to incorporate them into the present set of indicators.

## X. CONCLUSION

As an indication of improvements in environmental quality over time, the TRI Human Health and Ecological Indicators provide the EPA with a valuable tool to measure general trends related to impacts of TRI chemicals. They do not capture all environmental releases of concern, and thus changes in these indicators over time cannot be used to evaluate changes in other sources of environmental pollution. These indicators do, however, generally relate changes in releases to relative changes in chronic human health and ecological impacts from a large number of toxic chemicals of concern to the Agency. Importantly, the indicators also provide an ability to analyze the relative contribution of chemicals and industrial sectors to important changes in the indicators over time.



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## XI. REFERENCES


Hahn, R. and A. McGartland. 1989. The political economy of instrument choice: an examination of the U.S. role in implementing the Montreal Protocol. Northwestern University Law Review 83 (3): 597.

O'Bryan, T.R. and R.H. Ross. 1988. Chemical Scoring System for Hazard and Exposure Identification. Journal of Toxicology and Environmental Health, 1:119-134.

U.S. Environmental Protection Agency (EPA). 1985. Exposure to Airborne Contaminants Released from Land Disposal Facilities -- A Proposed Methodology. Prepared for the Office of Solid Waste by Environmental Science and Engineering, Inc. ESE Document Number 85-527-0100-2140. August.

U.S. Environmental Protection Agency (EPA). 1986a. Guidelines for Carcinogen Risk Assessment. 51 Federal Register 33992 (September 24, 1986).

U.S. Environmental Protection Agency (EPA). 1986b. Guidelines for Mutagenicity Risk Assessment. 51 Federal Register 34006 (September 24, 1986).

U.S. Environmental Protection Agency (EPA). 1986c. Report to Congress on the Discharge of Hazardous Wastes to Publicly Owned Treatment Works (the Domestic Sewage Study). Office of Water Regulations and Standards. EPA/530-SW-86-004. February.

U.S. Environmental Protection Agency (EPA). 1987a. Municipal Solid Waste Combustion Study Report to Congress. Office of Solid Waste. EPA/530-SW-87-021a. June.

U.S. Environmental Protection Agency (EPA). 1987b. Graphical Exposure Modeling System (GEMS) User's Guide. Prepared for the Office of Pesticides and Toxic Substances, Exposure Evaluation Division by General Sciences Corporation under Contract No. 68023970. February.

U.S. Environmental Protection Agency (EPA). 1987c. Integrated Risk Information System Supportive Documentation. Volume 1. Appendix A. Office of Health and Environmental Assessment, Office of Research and Development. EPA/600/8-86/032a. March.

U.S. Environmental Protection Agency (EPA). 1988a. Methodology for Evaluating Potential Carcinogenicity in Support of Reportable Quantity Adjustments Pursuant to CERCLA Section 102.

U.S. Environmental Protection Agency (EPA). 1988b. Report to Congress: Solid Waste Disposal in the United States. Volume 2. April.

U.S. Environmental Protection Agency (EPA). 1988c. National Survey of Solid Waste (Municipal) Landfill Facilities. Office of Solid Waste. EPA/530-SW88-034. September.

U.S. Environmental Protection Agency (EPA). 1988d. "Industrial Subtitle D Risk Screening Analysis Results." Prepared for the Office of Solid Waste by ICF, Inc., December 30.

U.S. Environmental Protection Agency (EPA). 1989. Proposed Amendments to the Guidelines for the Health Assessment of Suspect Developmental Toxicants. 54 Federal Register 9386 (March 6, 1989).

U.S. Environmental Protection Agency (EPA). 1990a. Exposure Factors Handbook. Office of Health and Environmental Assessment. EPA/600/8-89/043. March.

U.S. Environmental Protection Agency (EPA). 1990b. Policy Options for Stabilizing Global Climate: Report to Congress. Main Report. Prepared by the Office of Policy, Planning and Evaluation. EPA Document No. 21P-2003.1. December.

U.S. Environmental Protection Agency (EPA). 1992. User's Guide for the Industrial Source Complex (ISC2) Dispersion Models. Volume 2. Description of Model Algorithms. Prepared for the Office of Air Quality, Planning and Standards, Technical Support Division. March.



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# Appendix A

# Survey of Ranking and Scoring Systems

## I. Survey of EPA Scoring and Ranking Efforts

Scoring and ranking of chemicals is not a new undertaking. Numerous efforts have focussed on categorizing and ranking chemicals for a number of purposes. The most common purpose is devising a methodology to choose from among a vast number of chemicals those that merit further scrutiny. The following is a review of sixteen EPA scoring and ranking systems that have been or are used by OTS and other Agency Offices.

### A. OTS Efforts

#### 1. Screening Methodology for Pollution Prevention Targeting

USEPA (date unknown), Prepared for the Office of Toxic Substances

The Office of Toxic Substances prepared a screening methodology as a tool for targeting chemicals for pollution prevention. A three step scoring system, based on the toxicity (both potency and type of risk posed) and on the release/production ratio of the chemical, was used. Several risk classifications were evaluated; within each classification, a chemical was given a preliminary score of 3, 2, or 1 for high, medium, or low concern, respectively. The first risk area evaluated was cancer potency. All chemicals designated as B2 carcinogenic were given a preliminary score of 3 (high). Oncogenicity received an additional weighting factor of 3 to arrive at a raw score for cancer potency. General chronic toxicity and ecotoxicity were scored; these scores were given an overall weighting factor of 2. Reproductive effects, neurotoxicity, and developmental toxicity were also scored, but these scores were given a weighting factor of 1. The raw scores for all four risk groups were added together and multiplied by the release/production ratio to arrive at a composite score. For each chemical the composite score was calculated as:

$$CS_i = (O_i \cdot 3 + RDN_i \cdot 1 + C_i \cdot 2 + E_i \cdot 2) \cdot \frac{Release_i}{Production_i}$$

where:

| | | |
|---|---|---|
| $CS_i$ | = | Composite score for chemical *i* |
| $O_i$ | = | Oncogenicity concern for chemical *i* |
| $RDN_i$ | = | Reproductive, developmental,neurotoxicity concern for chemical *i* |
| $C_i$ | = | Chronic toxicity concern for chemical *i* |
| $E_i$ | = | Ecological toxicity concern for chemical *i* |

This methodology was used for internal EPA chemical targeting. It has not been, to our knowledge, publicly reviewed.

Pros: Method is simple. Broadly accounts for potency and severity of risk posed. Having three broad categories of potency allows the use of structure-activity and professional judgment to score chemicals lacking extensive toxicological databases. Includes consideration of both cancer and noncancer effects.

Cons: Method groups chemicals very broadly, limiting the variation in potencies that can be expressed. Method ranks chemicals ordinally, not proportionately, which does not allow for accounting of the magnitude of differences among the chemicals. Does not have an exposure component. Assumes that carcinogenic effects are more serious than reproductive effects. To our knowledge, method has not been reviewed outside of the Agency.

2. TSCA's TRI Chemical Risk Assessment Pre-screening Methodology

USEPA (date unknown), Memo from the Office of Toxic Substances (date unknown)

The objective of this exercise was to select the most likely candidates among TRI chemicals for possible regulation under TSCA. Of the 309 TRI chemicals, 193 were eliminated outright because they were already being assessed or regulated by another EPA division, they were not subject to TSCA, or no reports of use were received by EPA.

The remaining 116 chemicals were preliminarily ranked by exposure assessment and hazard assessment. The two assessments were used in concert with the investigators' knowledge to judge which chemicals presented the most significant risks to human health. This group of roughly 20 chemicals received top priority for more extensive and rigorous investigation, including exposure and hazard assessments, to determine which of them should be considered for regulation under TSCA.

Preliminary Exposure Ranking

One hundred sixteen TRI chemicals were ranked using the Exposure Scoring System for Existing Chemicals. The system was used to rank each chemical in four pathways: surface water (drinking water), environmental (aquatic organisms), ambient air, and groundwater. These rankings were not combined in a final ranking. To perform the rankings, two measures were estimated in each pathway for each chemical.

The first measure, potential of exposure, is a measure of the presence of the chemical in the environment. If the chemical is not expected to be released to a particular pathway, it is assigned a score of "none" for no potential of exposure. Otherwise, if the chemical does not exceed thresholds for physical and chemical properties (half-life, Henry's Law constant, vapor pressure), it is assigned a "low" or "none". Those that are expected to be released in a particular pathway and exceed the thresholds are assigned "high", "medium", or "low" potential of exposure depending on the level of potential exposure that is calculated by the

program. This calculation is a function of release and concentration levels at sites. Rough estimates are used if only partial information is available.

The second measure, population, is a score of the number of people that might be exposed to the chemical. It is calculated for each pathway and chemical. The system simply adds up the populations surrounding production sites, or if exposure mostly occurs during industrial use, extrapolates exposed populations from the number of industrial use sites. The final "high/medium/low/none" score is based on population thresholds.

The final score for each pathway area uses the following determination matrix:

| Final Exposure Score | | Population Measure | | | |
|---|---|---|---|---|---|
| | | High | Medium | Low | None |
| Exposure Measure | High | High | High | Medium | None |
| | Medium | High | Medium | Low | None |
| | Low | Medium | Low | Low | None |
| | None | None | None | None | None |

**Preliminary Hazard Ranking**

EPA intended to develop a Hazard Ranking System to rank the TRI chemicals based on measures of toxicity. However, only a preliminary search system was developed. It allowed the user to score all TRI chemicals that fit given criteria, e.g. all those with an RQ over 1000 lbs. This system was used to develop simple lists of high toxicity chemical groups. Using this information and their best judgement, the pre-screeners selected roughly 30 chemicals which they determined to be the most hazardous.

Note that this ranking system has only been used within EPA's Office of Toxic Substances and has not been publicly reviewed.

Pros: Exposure screening includes four pathways of exposure. Modelling approach is used to evaluate exposure potential. Population surrounding TRI site is also included as a measure of exposure potential.

Cons: Although modelling is used for exposure evaluation, the results are used to group the chemicals into low, medium and high exposure potential groups. Pathway-specific scores are not combined, thus requiring further judgments to evaluate overall exposure potential of a chemical. To our knowledge, method has not been reviewed outside of the Agency.

3. Chemical Scoring System for Hazard and Exposure Identification

O'Bryan, T. R. and Ross, R. H. (1988) Journal of Toxicology and Environmental Health, Vol (1):119-134

This system was developed by the Office of Toxic Substances and by the Oak Ridge National Research Laboratory. It combines expert judgement and objective scores to screen chemicals for further investigation for potential regulation under TSCA. Chemicals are scored in eleven areas:

| | |
|---|---|
| Oncogenicity | Genotoxicity |
| Developmental toxicity | Acute and chronic mammalian toxicity |
| Aquatic toxicity | Bioconcentration |
| Chemical production volume | Occupational exposure |
| Consumer exposure | Environmental exposure |
| Environmental fate | |

Scores are assigned by and reconciled between two independent experts. While the scores are based on delineated parameters, they can be adjusted in accordance with expert opinion. Scores for oncogenicity, genotoxicity, developmental toxicity and the exposure measures are based on weight-of-evidence. Scores for the others are based on thresholds (e.g. a bioconcentration score of 9 is assigned for BCF levels above 1000.) Tables 1 through 3 in our August 26 memorandum delineates the numerical ranges that comprise these scoring methods. In some cases, structure activity relationships were used to supplement available data. Individual scores generally range from 0 to 10 and are intended for comparison across areas and chemicals but not as weights for the calculation of a final chemical score. In fact, the methodology does not develop a final score. Instead, the scores from all eleven areas are presented as a score profile to which expert judgement is applied to determine whether a chemical presents a great enough hazard to undergo further investigation under TSCA. Note that this methodology has been published in a peer-reviewed journal.

Pros: System considers a large number of health endpoints (cancer, developmental toxicity, genotoxicity) in the evaluation. Makes use of both available data and expert judgment, allowing for coverage of a large number of chemicals. Published in a peer-reviewed journal.

Cons: System does not combine scores for overall judgment on relative toxicity of a chemical. In fact, the method explicitly states that scores can be used for comparisons across areas, but are not intended as weights for combination into a final score. Method does not include an exposure component.

4. CERCLA Section 104 "Third Priority List" of Hazardous Substances that will be the Subject of Toxicology Profiles

USEPA 1990, Prepared for the Office of Toxic Substances, February

EPA is using this system to select and rank the 275 most hazardous chemicals from among all substances found at National Priority List sites. Three principal criteria determine how hazardous a chemical is: 1) frequency of occurrence at NPL sites, 2) chemical toxicity, and 3) potential for human exposure. Measures of these criteria are used to calculate site and exposure ranks for each chemical, which determine the chemical's final ranking.

Frequency of occurrence is measured as the percent of sites at which the chemical is known to occur. Toxicity of the chemical is measured by its Reportable Quantity (the lowest of the mammalian, acute and chronic toxicity RQs was used.) When these ratings were not available, the chemical was assigned an RQ equivalent by the EPA Structure Activity Team. A site index was calculated for each chemical as:

$$\text{Site Index} = \frac{\text{Frequency of occurrence (percent)}}{\text{RQ}}$$

The chemicals were assigned ordinal site ranks beginning with 1 for the chemical with the highest site index, 2 for the chemical with the next highest site index, etc.

The measurement of chemical exposure is considerably more involved. First, an exposure index value is calculated for each chemical as:

$$\text{Exposure index} = \text{WCR} + \text{WFR} + \text{SCR} + \text{SFR} + (2 \times \text{BPR})$$

where:

| | | |
|---|---|---|
| WCR | = | the geometric mean of chemical concentration in water at all sites where the chemical occurred, ranked ordinally |
| WFR | = | percent of sites at which the chemical occurred in water / percent of sites at which the chemical occurred in any media, ordinally ranked |
| SCR | = | the geometric mean of chemical concentration in soil at all sites where the chemical occurred, ranked ordinally |
| WFR | = | percent of sites at which the chemical occurred in soil / percent of sites at which the chemical occurred in any media, ordinally ranked |
| BPR | = | boiling point of the chemical, ordinally ranked |

For WCR, the geometric mean as indicated is calculated for each chemical. The chemicals are then ranked ordinally according to this value; WCR equals the rank assigned to the chemical.

This method holds for each of the five variables listed above. Note that boiling point values are used as a correlate of potential for air migration.

Because NPL site concentration data are not available for many chemicals, a second methodology to calculate exposure was developed to complement the first. This method takes advantage of the fact that a chemical's status as a chemical of concern gives some indication of the chemical's exposure potential. Thus chemicals were ranked ordinally by the number of NPL sites at which they were listed as chemicals of concern. The lesser of this measure and the exposure index described above was used as the exposure rank.

Finally, these ranks were adjusted based on existing exposure information compiled in six data bases: NRC, AHE, DOT/HMIS, NEXIS, NHATS and RTS. Because of source and methodological disparities between the databases, the data they contained were not in themselves useful. However, because the simple occurrence of a chemical in one of the databases implies some degree of exposure, the number of databases in which a chemical was listed was used to determine the adjustments made to the exposure ranks. (Note that because the first four databases contained data from overlapping sources, multiple occurrences of a chemical in these databases was taken as a single listing.) The adjustment was made as follows. The exposure rank was multiplied by a factor of 0.9 if a chemical was listed in only one database, by 0.8 if in two databases, and by 0.7 if in three databases.

The site and exposure ranks of each were combined using the following formula:

$$\text{Hazard Index} = 2/3 \times \text{Site Rank} + 1/3 \times \text{Exposure Rank}$$

The weights reflect the fact that the site rank represents two of the three principal criteria mentioned initially, while the exposure rank represents only one. The chemicals were assigned final ordinal hazard ranks beginning with 1 for the chemical with the lowest hazard index, 2 for the chemical with the next lowest site index, etc.

Pros: Uses a peer-reviewed, well-established measure of relative toxicity (RQ) for toxicity ranking. Combines all measures (toxicity, exposure, frequency of occurrence) into a single index for each chemical.

Cons: Exposure component relies on availability of site-specific concentration data for exposure potential evaluation, which is not available for our purposes. Toxicity and exposure ranked ordinally, so that proportional differences in potency and exposure potential are not captured. Use of RQ also does not capture severity of effects.

5. Toxic Chemical Release Inventory Risk Screening Guide

(USEPA 1989, Prepared by the Office of Toxic Substances, Volume 1, July)

The Risk Screening Guide serves to explain both the meaning of Toxic Release Inventory (TRI) data and ways of interpreting that data. Volume One of the document is divided into five sections. The first section details the advent of the TRI program as well as the nature of, limitations on, and modes of access to the TRI data. Section Two details and explains the elements of risk assessment. Section Three presents the guide's qualitative methodology for risk assessment for each exposure route, incorporating the elements detailed in Section Two. Section Four proposes options for acting on the results of the assessment and Section Five lists a host of resources that can be used to answer any further questions.

The Risk Screening System presented in Section Three merits special attention. The system centers itself around qualitative measurements of different chemical-specific and site-specific factors. The user of the system first selects an exposure route (either air, land, surface water or POTW). The next step is to record the location of release, the zones of effect (inner and outer), and the population of interest. The user then delineates different "exposure factors" which depend upon the exposure route chosen (i.e. wind direction for air or bioconcentration factors for surface water). The scores for these factors depends upon the factor being discussed. For example, a water discharge receives a "+" if it flows to a small lake or stream and a "-" if it flows to a large body of water. Next, the user should select a toxic measure for each chemical from among a set of measures presented in Appendix A (discussed below). The user selects the lowest ranking among all of the different toxicological ranks. Next, the quantity of release should then be listed as either "high," "moderate," or "low" through the use of data presented in Appendix C. The user compares the releases as recorded in TRI to either the table of median emissions or by to local releases. Exposure factors should then be recorded as detailed in Appendix D (discussed below), including high/low environmental transformation, release rate, and any other factors which may seem relevant.

The result of the risk screening system is a profile of scores. From this information it is possible to assess the relative severity of industrial practices in the area. The user can consult local experts in order to get a feel for the individual risk.

Volume Two includes appendices which provide data and examples to facilitate the assessment process. Appendix A ranks toxicological information on chemicals according to the following scheme:

| Toxicological Measure | Group 1 | Group 2 | Group 3 |
|---|---|---|---|
| TPQ (lbs.) | 1 10 100 | 500 | 1,000 10,000 |
| RQ (lbs.) | 1 10 100 | 1,000 | 5,000 |
| RfD (mg/kg-day) | < 0.01 | 0.01 - 0.1 | > = 1.0 |
| WQC (mg/L) | < 1 | 1 - 10 | > = 10 |
| Cancer Potency | All | | |

These ranking boundaries are used for each of the RQs (aquatic, chronic, acute, and carcinogenic), RfDs (inhalation and oral), and WQCs (chronic and acute).

Appendix B aids users in assessing air releases. It discusses a generic air modelling exercise which uses the Industrial Source Complex Long-Term (ISCLT) model. It provides two graphs which display the results of generic model runs, the first plotting concentration versus distance from the release site for various stack heights, and the second plotting concentration versus distance from the release site for various durations of release. Multiplying data points on the graph by the actual release quantities provides an estimate of the concentration at different distances of concern.

Appendix C assists users in assessing the severity of chemical releases. It provides information on median chemical release data and actual TRI chemical release data (classified by SIC code) to assist in assigning a "severe," "moderate," or "low" score to the quantity of release (see the discussion on the Risk Screening System in Volume One).

Appendix D provides information on environmental fate characteristics of different chemicals to provide rankings. The characteristics used to evaluate fate in different environmental media and their rankings are listed below:

| Factor | Measure | High Concern (+) | Low Concern (-) |
|---|---|---|---|
| Volatilization | Henry's Constant (atm-$m^3$/mol) | ≥ $10^{-2}$ | ≤ $10^{-6}$ |
| Leaching & Soil Mobility | $Log_{10}$ ($K_{oc}$) | ≤ 1.5 | ≥ 4.5 |
| Bioconcentration | BCF | ≥ 1,000 | ≤ 250 |
| Air Abiotic Persistence | Atmospheric Half-life | ≥ 1 year | ≤ 1/2 day |
| Water Abiotic Persistence | Aquatic Half-lives | ≥ 1 year | ≤ 1/2 day |
| Air Biotic Persistence | Degradation Rate | many months to years | 1 to 7 days |
| Water Biotic Persistence | Degradation Rate | many months to years | 1 to 7 days |
| Biological Treatment | Rate of removal in bio. treatment | $Log_{10}$ ($K_{ow}$) ≤ 1.5<br>$H_c$ ≤ $10^{-5}$<br>resistant to degr. | rapidly removed:<br>-P for phys/chem<br>-B for biodegr. |

The measure for water abiotic persistence stems from the longest of the hydrolysis, direct photolysis, and indirect photoreaction.

Appendix H presents and describes the Roadmap database as well as other databases that contain information on Section 313 chemicals. The Roadmap database includes the following information for each chemical in tabular form:

- Federal regulations that apply to the chemical, along with relevant regulatory levels
- States that have drinking water standards or recommendations, along with relevant regulatory levels, as reported in the Federal-State Toxicology and Regulatory Alliance Committee (FSTRAC)
- States that have ambient air information, including ambient air standards or guidelines, pollutant research information, source testing information, monitoring data, emissions inventory information, and permitting information, as reported in the National Air Toxics Information Clearinghouse (NATICH).

- States that have water monitoring information, as reported in the Storage and Retrieval Systems (STORET).

- General sources of information, including on-line data bases, and documents from EPA and other sources.

This appendix includes expanded descriptions of these information sources. ROADMAPS has since been updated to include additional data. Its "Carcinogenicity Matrix" inclu 's results from the National Toxicology Program bioassay tests (either positive or negative .or carcinogenicity); the National Toxicology Program's carcinogenicity ranking; the carcinogenicity rating assigned by the International Agency for Research on Cancer; the EPA's carcinogenicity rating; and the GENETOX carcinogenicity evaluation. It also now contains a "Health and Environmental Effects" table which indicates whether a chemical is at a level of concern for heritable mutations, developmental toxicity, reproductive toxicity, acute toxicity, and chronic toxicity, as well as the references for this data (among EPA databases).

The remaining appendices contain other information to guide a use through the risk assessment process. Appendix E presents information concerning the different types of releases, the release frequency, existing controls, and estimation methods for the releases. Appendix F presents a case study using the risk screening method (described below). Appendix I presents a sample EPA Hazardous Substance Fact Sheet. Each of these sheets discusses one of the Section 313 chemicals, providing information on typical modes of exposure, means of protection, proper handling, etc. Appendix J provides an example of an EPA Chemical Profile which provides physiochemical information on the Section 313 chemicals and which also discusses topics covered on the EPA Hazardous Substance Fact Sheet.

Pros: Appendix A of the Risk Screening Guide allows grouping of chemicals according to any of five measures of toxicity; using alternative measures of toxicity allows a larger number of chemicals to be scored than if only a single measure was used. Appendix D groups chemicals into groups of "high concern" and "low concern" based on environmental fate characteristics. The Risk Screening Guide has been peer reviewed and is published.

Cons: The grouping approach allows only broad characterization of toxicity and exposure, and does not consider severity or potency. Exposure evaluation does not explicitly consider populations (although this can be considered on a site-by-site basis).

## B. Other Agency Scoring Systems that Use TRI Data

### 1. Targeting Pollution Prevention Opportunities Using the 1988 Toxics Release Inventory

USEPA 1990, Prepared for the Office of Policy, Planning and Evaluation, Pollution Prevention D ision, September 29)

OPPE's Pollution Prevention Division (PPD) developed a method to rank chemicals and facilities based on total volume of a subset of TRI chemicals. A list of high-priority chemicals was established for air, land, and water releases based on toxicity and exposure potential (based on the mobility of the chemical) in the TRI Risk Screening Guide. After a list was established for each media, the release volume of those chemicals became the ranking instrument. While no exposure-based adjustments were actually made to the rankings, possible methods for such adjustments were discussed in some detail in the text. The population considered at risk for each pathway varies by the mobility of the chemical. Thus, only populations relatively close to the facility are considered for low mobility chemicals, while at greater distances are included for high mobility chemicals. The table below shows how distance from facility and chemical persistence affect PPD choice of populations. PPD also proposed a method to adjust for the exposure potential of aquatic ecosystems for discharges to surface waters. Similar to human populations within circles of given radii from the facility, the stream volume acts as a proxy for aquatic exposure. The water-volume proxy assumes that densities and types of aquatic organisms are constant among all streams and are strongly positively correlated with total volume of water. Proposed methods for accounting for ecological risk from discharges to other media were resource intensive and did not lend themselves to computer automation.

This method was used for internal EPA chemical evaluation and has not been publicly reviewed.

**Concentric Ring Radius From Facility For Population Count**

| | Mobility of Chemical | | |
|---|---|---|---|
| Pathway | High | Medium | Low - No Data |
| Point and Non-Point Air Release | 4 miles | 2 miles | 1 mile |
| Underground and Land Releases | 1 mile | 1/2 mile | 1/4 mile |
| Surface Water Releases | 15 miles | 10 miles | 5 miles |

Note: Surface water distances are downstream distances from the facility.

Pros for exposure evaluation: Combines Risk Screening Guide environmental fate groupings with simple rules for defining the size of the potentially exposed population. This is a straightforward approach that allows quick, rough weighting of emissions by potential exposure.

Cons for exposure evaluation: Does not consider factors affecting differences in media concentrations among sites as part of exposure evaluation. Selection of distances to consider for exposed population is somewhat arbitrary.

**2. Ranking the Relative Hazards of Industrial Discharges to POTWs and Surface Waters**
USEPA 1991, Prepared for the Office of Policy Analysis, February 4

The Office of Policy Analysis developed a population weighted hazard index that ranked water bodies and POTWs reported in TRI. OPA used Reportable Quantities as proxies for three risk classes for which ranks were provided. Cancer potency, chronic toxicity, and aquatic toxicity were treated separately in deriving indexes and ranks. For each risk class, each chemical release was divided by the RQ for that risk class. The weighted releases were summed over a selected set such as state or county to arrive at an unadjusted index.

The equation for calculating the unadjusted Hazard Index is:

$$H_i = \sum \frac{R_x}{RQ_x}$$

where:

$H_i$ = Hazard Index for set *i*
$R_x$ = Pounds released of chemical *x*
$RQ_x$ = Reportable Quantity for chemical *x*

For each state or county, unadjusted indices were calculated for cancer, chronic, and aquatic toxicity. The indices for cancer potency and chronic toxicity were adjusted using the size of the exposed population to reflect human exposure potential:

$$H_i = \sum \frac{R_x}{RQ_x} \cdot P$$

where:

P = Persons per square mile in the county of release $R_x$

Aquatic toxicity indices were not adjusted using this method due to inadequate data about the size of the exposed aquatic population. Thus, the OPA work does not address the difficult question of adjusting indices based on exposure potential to aquatic life and habitats.

For releases to POTWs, the analysis addressed the hazard of POTW residuals as well as effluent. Average removal rates were applied to chemicals released to POTWs. Standard partitioning rates were applied to the portion removed by the POTW. Hazard indices were then generated for each partitioning pathway (sludge, volatilization) within the POTW.

This methodology was used within the EPA and has not been publicly reviewed.

Pros: Uses peer-reviewed, publicly available toxicity measure (RQs) that are available for a fairly large percentage of TRI chemicals. Also considers county population density as a surrogate measure of exposure potential.

Cons: Does not consider environmental fate of chemicals in exposure evaluation. Use of RQs does not include consideration of severity of effects. RQs do incorporate some consideration of potency, but groupings according to potency are broad.

3. Review of Region VII TRI Strategy

USEPA 1991, Memo from Dermont Bouchard, EPA Region VII to Loren Hall, OTS, July 9

Region VII is developing strategies to utilize TRI data. One strategy ranks geographic areas by human health and aquatic ecological risks to determine areas most in need of investigation for further enforcement, remediation, technical assistance, or other purposes. The human health risk analysis, which is separate from the ecological risk analysis, is measured by relative daily toxic loadings (RDTLs). For a given site, an RDTL is estimated for the following categories:

Non-cancer acute toxicity by ingestion
Chronic inhalation cancer
Chronic ingestion cancer
Chronic inhalation non-cancer
Chronic ingestion non-cancer

A toxicity measure (for example, the inverse of the RfD for chronic ingestion non-cancer) is multiplied by the site loading to the appropriate media (surface water emission in this case) for each category. These RDTLs are not to be added, unless they are added within a category across the various chemicals present at a site. Because RDTL units are different for each category, they are comparable across sites only within categories.

Aquatic ecological risk for a site is determined in a similar manner. A multi-trophic analysis is used to identify an $LC_{50}$ that is the lowest, most protective value for the site. The RDTL is calculated as:

RDTL = chemical loading volume X $LC_{50}$ / stream volume

Total risk for a site is the sum of the RDTLs across chemicals released at that site.

The Region VII TRI strategy is currently under peer review within the EPA.

Pros: Considers acute and chronic toxic endpoints and multiple exposure pathways. The toxicity measures used (RfDs, $q^*$, WQC) reflect the relative potencies of chemicals. For ecological risk, more than one trophic level is considered.

Cons: Scores are not combined across sites for a single chemical index; however, scores may be combined within a single site. The human health evaluation categories do not consider environmental fate or population exposure potential. This system is oriented more toward identifying problem sites than in characterizing overall risk from all sites.

## C. OSWER Scoring and Ranking Systems

### 1. Hazard Ranking System: Final Rule

55 Federal Register No. 241, pp. 51532-51667, December 14, 1990

The Hazard Ranking System (HRS) is the principal mechanism used by the EPA to place sites on the National Priorities List (NPL). It provides a methodology for scoring a site based on various site characteristics. It incorporates information representing four exposure pathways: ground water, surface water, soil and air. If the site's score exceeds an established threshold, the site qualifies for the NPL.

## Hazard Ranking Score

The hazard ranking score is calculated as:

$$HRS = (S^2_{gw} + S^2_{sw} + S^2_{s} + S^2_{a})^{1/2}$$

where:

S = is the scores for each of the four pathways delineated below.

Using the root-mean-square calculation, low migration pathways scores yield a low HRS. However, the HRS score could be relatively high even if only one pathway score was high. This is an important requirement for HRS scoring because some extremely dangerous sites pose threats through only one migration pathway.

While the scoring system for each pathway is quite sophisticated, the pathway scores follow this general methodology:

Likelihood of Release x Quantity of waste at the site x Measure of toxicity x Measure of exposure

The pathway scoring systems demonstrate how toxicity and exposure characteristics can be scored (i.e. weighted). They are much more sophisticated than ordinal scoring systems that implicitly weight characteristics without any underlying justification.

## Ground Water Migration Pathway

The pathway score is the product of the following three categories (divided by a scaling factor of 82,500) for the aquifer and contaminant yielding the highest pathway score.

| Likelihood of Release | X | Waste Characteristics | X | Targets |
|---|---|---|---|---|
| Highest of:<br>Observed release = 550<br>or<br>Potential to release =<br>Contaminant Score x<br>(Net precipitation score +<br>Depth to aquifer score +<br>Travel time score) | | Score of [(Score of<br>Toxicity score and<br>Mobility score) x<br>Weighted Hazardous waste<br>quantity] | | Nearest well score +<br>Weighted Population +<br>Resources score +<br>Wellhead score |

The scores for these individual components are assigned based on conditions set by the Rule. For example, the contaminant score is 10 if a liner is not present in the

containment system, 9 if one is present. The toxicity score is the highest of 1) chronic toxicity score based on ranges for RfDs, 2) carcinogenicity score based on ranges for human carcinogenicity slope factors and weight-of-evidence, and 3) acute toxicity score based on ranges for oral $LD_{50}$, dermal $LD_{50}$, and various $LC_{50}$. Mobility is scored based on ranges for water solubility and the distribution coefficient (which is based on soil type) of the contaminant. Table 1 of our August 26 memorandum delineates the numerical ranges that compose this scoring method.

The numerous inputs for the groundwater pathway analysis include both chemical- and site-specific measures. Many of these measures are not available for the sites listed on the TRI (for example, chemical waste containment conditions or the characteristics of the geology of surrounding strata.) The following list delineates those measures that are available for many of the TRI chemicals and sites:

Chronic toxicity (human) RfD
Human carcinogenicity slope factor
Human carcinogenicity weight-of-evidence
Oral $LD_{50}$
Dermal $LD_{50}$
Dust or mist $LC_{50}$
Gas or vapor $LC_{50}$
Water solubility
Distribution coefficient $K_d$
Quantity or volume of waste
Population
Net precipitation
Depth to the aquifer
Nearest well

## Surface Water Migration Pathway

There are two components for likelihood of release, overland/flood and groundwater to surface water. Each is the higher of an observed or potential release. The component that yields the highest score when multiplied by the sum of the threat scores is the likelihood of release that is used in the HRS score for this pathway. Threats are composed of three categories: drinking water, human food chain, and environmental. The score of each threat is the product of the waste characteristics and targets for that threat.

As with the groundwater migration pathway, surface water migration pathway is based on scoring different conditions regarding site, pathway, environmental, chemical, quantity, and population characteristics. The internal scores are used as weights, not ordinal ranks, for these parameters. The methodology is designed so that worst case conditions determine the final HRS rank. Thus if two exposure routes within a media migration

pathway exist for a given site, the most damaging route (as scored) is used to calculate the rank. For example, if the risk of exposure through drinking water is worse than that through fish consumption, the surface water score for the site will be based on risks from drinking water.

The surface water migration pathway scoring system utilizes a combined rating factor to score combinations of toxicity and persistence of a chemical. The factor matrix scores twenty four combinations yielding scores that range eight orders of magnitude.

Like the analysis of the groundwater pathway, the surface water pathway analysis incorporates many measures that are not available for the sites listed on the TRI (for example, the area over which a chemical drains into the surrounding environment.) The following list delineates those measures that are available for many of the TRI chemicals and sites:

Quantity or volume of waste
Chronic toxicity (human) RfD
Human carcinogenicity slope factor
Human carcinogenicity weight-of-evidence
Oral $LD_{50}$
Dermal $LD_{50}$
Dust or mist $LC_{50}$
Gas or vapor $LC_{50}$
Half-life in water from combined effects of:
- hydrolysis
- biodegradation
- photolysis
- volatilization

Log $K_{ow}$
Stream volume in cubic feet per second
BCF
EPA chronic and acute Ambient Water Quality Criteria
EPA chronic and acute Ambient Aquatic Life Advisory Concentrations
Population

Air Migration Pathway

The methodology for this pathway considers gas releases and particulate releases separately. A site which has both kinds of releases is assigned an air pathway score based on whichever kind of release poses the higher risk (as determined by this methodology.) As with the two pathways described above, a release score is based either on an observed release, if present, or on the potential of the site to release. The release score is multiplied by the waste characteristic score and the target score to yield the overall pathway score.

The air water migration pathway methodology is based on scoring different conditions regarding site, pathway, environmental, chemical, quantity, and population characteristics. Specifically, the waste characteristic score comprises measures of toxicity, mobility, and quantity of the chemical released. The target score comprises measures of the nearest individual, surrounding population, natural resources and sensitive environments. Many of the criteria on which scores of these qualities are based are not appropriate for the TRI indicator methodology (e.g. acreage of a nearby sensitive wetland environment.) However, many physical and chemical properties of the chemicals are used as criteria to measure toxicity, mobility, and migration potential. The numerical ranges of these criteria are presented in our August 26 memorandum.

As with the groundwater and surface water migration pathways, internal scores of the air migration pathway are used as weights, not ordinal ranks, in the calculation of the pathway score. In addition, as with the other pathways, the air pathway methodology is designed so that worst case conditions determine the final HRS rank.

Like the analyses of the first two pathways, the air migration pathway analysis incorporates many measures that are not available for the sites listed on the TRI (for example, containment measures in effect and their degree of effectiveness.) The following list delineates those measures that are available for many of the TRI chemicals and sites:

Vapor pressure
Henry's constant
Quantity or volume of waste
Chronic toxicity (human) RfD
Human carcinogenicity slope factor
Human carcinogenicity weight-of-evidence
Oral $LD_{50}$
Dermal $LD_{50}$
Dust or mist $LC_{50}$
Gas or vapor $LC_{50}$
Population

Note that this ranking system has been published in the Federal Register and has been publicly reviewed.

Pros: A reviewed and published method for evaluating and ranking hazardous waste sites. Evaluates four exposure pathways and adds the scores to yield a single site score. Considers many relevant site and chemical characteristics when scoring exposure. Toxicity score is based on highest of cancer, noncancer and acute toxicity subscores, thereby incorporating consideration of a range of health endpoints. Scores are used as weights, not ranks, so magnitude of exposure and toxicity can be considered.

Cons: Exposure evaluation requires much more detailed site-specific data than are available for TRI sites.

2. Application of the Hazard Ranking System to the Prioritization of Organic Compounds Identified at Hazardous Waste Remedial Action Sites

Hallstedt, P. A., Puskar, M. A., and Levine, S. P (1986) Hazardous Waste and Hazardous Materials, Vol (3):2, pp. 221-232

This system ranks chemicals by relative risk to target those chemicals that are of highest concern with respect to hazardous waste cleanup and the reduction of hazards to human health. The authors' measure of relative risk incorporates the methodology of the first (unrevised) EPA Hazard Ranking System to score chemical toxicity and persistence.

The risk formula that determines the ranking score is straightforward:

Score = Measure of Hazard X Exposure

The measure of hazard is based on a chemical's toxicity and persistence characteristics. Each characteristic is ranked from 0 to 3, 3 representing the highest order of toxicity or persistence. The methodologies underlying these rankings are referenced and can be explored if necessary. The overall measure of hazard reflects a synergistic effect between toxicity and persistence and is summarized in the following table:

| Measure of Hazard | | Persistence | | | |
|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 3 |
| Toxicity | 0 | 0 | 0 | 0 | 0 |
| | 1 | 3 | 6 | 9 | 12 |
| | 2 | 6 | 9 | 12 | 15 |
| | 3 | 9 | 12 | 15 | 18 |

Exposure is measured as the percentage of the sample sites that release a chemical weighted by the concentration of each release. Thus, exposure is not an absolute measure of population exposure but a relative measure that is a function of the sample of sites that is used. Concentration of release was used in lieu of volume of release, because data on the latter was unavailable.

Note that this methodology has been published in a peer-reviewed journal.

Pros: Simple, straightforward assignment of chemicals to categories based on toxicity and persistence. Provides relative ranks of chemicals based on toxicity-persistence matrix. Allows for categorization of large number of chemicals, based on available data, SAR, and Best Professional Judgment. Has been published in peer review journal.

Cons: Broad groupings do not permit refined accounting of relative toxicity or persistence of chemicals. Exposure component inappropriate for our purposes, since it considers only the frequency of occurrence of chemicals, and not their concentrations or volumes. Populations exposed are not considered.

## D. Office of Water Scoring and Ranking Systems

### 1. A Ranking System for Clean Water Act Section 307(a) List of Priority Pollutants

USEPA 1985, July 3 (Office unknown)

This methodology was developed to determine which chemicals should be added to or subtracted from the Priority Pollutants List, a list of chemicals that pose the greatest hazard to human health and the environment nationwide in surface water bodies. Chemicals are list candidates if they are either very toxic or exposed to a large population. This system does not attempt to rank chemicals, but simply provides the decision rule for inclusion or exclusion in the list. However, because the chemicals are scored in the process of determining exclusion or inclusion, this system is relevant to the ranking discussion. It is unknown whether this methodology has been peer-reviewed or made available for public comment.

To evaluate toxicity, the following five categories are considered, followed by the variables considered in each category:

1) Aquatic Toxicity
   acute ($LC_{50}$), chronic (MATC)
2) Mammalian Toxicity
   acute oral ($LD_{50}$), acute dermal ($LD_{50}$), chronic/sub-chronic (LDLo and TDLo)
3) Human Health
   Evidence of carcinogenicity, mutagenicity and teratogenicity
4) Bioaccumulation
   BCF, BAF, Log P
5) Environmental Persistence
   environmental half-life, hydrolysis rate, Henry's constant, KD value

Because the variables in a category are often well-correlated, they are considered together to avoid biasing the system by considering the same topic twice. A score is

developed for each category by considering the most potent effect of any of the variables in that category. For example, the scoring system for Aquatic Toxicity is:

| Score | Acute ($LC_{50}$) (mg/L) | Chronic (MATC) (mg/L) |
|---|---|---|
| 12 | <0.1 | <0.01 |
| 10 | 0.1 to 1.0 | 0.01 to 0.1 |
| 5 | 1.0 to 10.0 | 0.1 to 1.0 |
| 3 | 10.0 to 100 | 1.0 to 10.0 |
| 0 | >100 | >10 |
| * | Insufficient information | |

The values of the scores assigned to each category were based on expert judgment. The scoring systems are similar for the other categories. One of the advantages of this method is that data gaps in one variable may be filled by data from another within the same category. Note that in the Human Health category, weight of evidence classes, not numeric measures (such as $q^*$), are assigned score values. If the sum of the scores over the five categories is greater than 10, then the chemical is listed.

National exposure potential is evaluated in a similar manner. The following categories are individually scored on a scale of 0 to 10 based on numerical thresholds as above:

1) Amount of discharge nationwide (metric tons per year)
2) Number of sites of discharge having detectable concentrations
3) Frequency of detection in ambient waters (percent)
4) Frequency of detection in aquatic sediments (percent)
5) Frequency of detection in industrial or municipal effluents (percent)

If the sum of the scores over the five categories is greater than 10, then the chemical should be listed.

Pros: Considers a range of acute and chronic toxicities. Includes persistence and bioaccumulation. Allows for more than one measure to be used to rank a chemical within one category, thus allowing a wider range of chemicals to be scored. Allows use of expert judgment to fill in data gaps.

Cons: Toxicity ranks are ordinal, not proportional. Since this system was not intended for site-specific use, it is limited in its consideration of exposure potential; exposure potential is based only on environmental fate properties of the chemicals and frequency of occurrence.

## 2. Screening Procedure for Chemicals of Importance to the Office of Water

USEPA 1986, Prepared by the Office of Health and Environmental Assessment, November 14

This screening method was developed by ORD for the Office of Water to differentiate quickly and inexpensively between higher and lower risk chemicals so that the Office could set priorities for more intensive review of a small set of chemicals. Each chemical is identified as having "high", "low" or "unknown" toxicity and "high", "low" or "unknown" exposure. Chemicals are categorized using this matrix:

| Rank Categories | | Toxicity | | |
|---|---|---|---|---|
| | | High | Low | Unknown |
| Exposure | High | 1 | 2 | 2 |
| | Low | 3 | 4 | 4 |
| | Unknown | 3 | 4 | 4 |

A fifth and lowest category is reserved for chemicals that are clearly not an environmental problem. Chemicals in this category must either 1) have a half-life of less than a few minutes and not be highly toxic (acute only), 2) be easily treatable, or 3) have not been shown to be toxic at high concentrations.

The criteria for labeling a chemical as having "high" toxicity is different depending on the exposure pathway and exposed population. For example, a chemical exposed to human populations is "highly" toxic if it is a definite, probable or possible carcinogen, or it is developmentally toxic. A chemical exposed to aquatic life populations is "highly" toxic if $LC_{50}$ < 100 mg/l or chronic toxicity < 1 mg/l.

The criteria for labeling a chemical as having "high" exposure is also different depending on the exposure pathway and exposed population. Usually several conditions must be met. Among these, for example, are BCF thresholds and whether or not the chemical has been detected (at any level) in a relevant water pathway.

While "high" criteria are not comparable across pathways and populations, this method succeeds in grouping chemicals roughly by risk. Chemicals not labeled "high" for toxicity or exposure are labeled "low", unless information is unavailable. Data gaps are minimized by using chemical estimation models (ENPART, a fate model; CHEMFATE: CHEMEST.)

It is unknown whether this methodology has undergone peer review or public comment.

Pros: Quick, easy to understand. Assigns rank based on toxicity and exposure potential simultaneously rather than considering these elements separately. Allows scoring of a large number of chemicals based on available data, SAR, and Best Professional Judgment. Considers a range of health endpoints. Implicitly weights cancer and noncancer by automatically assigning "high" ranks to cancer and developmental toxicity.

Cons: Consideration of potency, severity and weight of evidence are implicit, not explicit, in assignment of chemical to one of the toxicity categories. Limited consideration of exposure, based on environmental fate properties and the frequency of detection in U.S. waters.

## E. Air Office Scoring and Ranking Systems

### 1. The Source Category Ranking System: Development and Methodology

USEPA 1990, Prepared for the Office of Air Quality Planning Standards, Chemicals and Petroleum Branch, February 16

This system was devised to rank sources of different emissions in order to prioritize air pollutant source categories. The scoring system looks at both long- and short-term effects of pollutants, taking into consideration pollutant concentrations, maximum and average exposure, the total exposed population, and health risks associated with the exposure. To our knowledge, this system has only been used internally by the EPA and has not been publicly or peer reviewed.

Health effects scores are based upon carcinogenicity, reproductive and developmental toxicity, acute toxicity data, and nonlethal health effects. Before calculating health risk scores, all health effects are scaled by dividing by the respective maximum health score so that the maximum equals one. Scores for a particular site are then added across pollutants.

Exposure scores were calculated using an algorithm integrated with the Industrial Source Complex Long-Term Model (ISCLT). Exposures per unit loss rates were calculated for both long-term (average) and short-term (peak) chemical releases. These were then scaled by dividing by the maximum exposure score such that the greatest exposure would equal one.

Pros: System was devised to rank air pollutant source categories. It utilizes data on acute and chronic toxicity, pollutant concentrations (as obtained from air modelling), populations exposed and human health risk. Scores are developed for carcinogenicity and other health end points. Scores are summed across pollutants to obtain source specific values. Normalizes scores by dividing each score by maximum value possible in that category.

Cons: System is media-specific to EPA's Air program. The system neither incorporates severity of health effects nor does it allow weight of evidence considerations in scoring.

Unknown if system has been peer reviewed. The system also does not include non-human health effects in establishing a source-specific score.

2. Measuring Air Quality: The New Pollutants Standards Index
USEPA 1978, Prepared for the Office of Policy Analysis, July

This index measures air quality based on the potential acute human health effects of five major pollutants: carbon monoxide, photochemical oxidants, nitrogen dioxide, sulfur dioxide, and particulate matter. The index is formed by calculating the following subindex for each pollutant:

$$\text{Subindex} = \frac{100 \text{ X Observed Concentration}}{\text{National Ambient Air Quality Standard (NAAQS)}}$$

The Index value (ranging from 0 to 500) is equal to the highest of the five subindices. The pollutant responsible for the highest subindex and all pollutants with subindices greater than 100 are named (a subindex greater than 100 indicates that the pollutant concentration violates the NAAQS.) Because of the limited definition, indices calculated in this way on a regional or local basis are not comparable because variables such as area of effect, duration of concentration, and exposed population are not controlled.

This index has been published and was designed specifically for public use.

Pros: This index provides a measure of overall air quality based on the potential acute human health effects of five criteria air pollutants. The index is simple and easy to understand. Subindices are calculated for each pollutant by dividing the observed concentration by the relevant National Ambient Air Quality Standard.

Cons: This index is severely limited to just the five criteria air pollutants. The index only incorporates acute health effects data along with ambient air concentration data. It does not look at chronic health effects, ecological effects, populations exposed, weight of evidence considerations, or severity of effects. Additionally, the index does not allow for combining values into a single score.

3. National Emissions Standards for Hazardous Air Pollutants for Source Categories: Proposed Regulations Governing Compliance Extensions for Early Reductions of Hazardous Air Pollutants

USEPA 1991, Prepared for the Office of Air Quality Planning Standards

This proposed rule will implement provisions of the Clean Air Act Amendments of 1990 that allow a source to obtain an extension for compliance with air emissions standards if the source has achieved an overall emission reduction of 90% or more by specified dates. Reductions are calculated based on overall emissions from the source; therefore, a source can use greater than 90% reductions from some pollutants to offset less than 90% reductions for other pollutants to achieve the overall 90% reduction. However, certain rules govern this practice of offsetting for "high-risk" pollutants. Offsetting of these "high-risk" pollutants with lower risk pollutants is calculated based on the relative toxicity of the chemicals. For carcinogens, weighting factors are applied to the emissions of these "high-risk" chemicals, so that every 1 pound of these carcinogens equals between 10 and 1,000,000 pounds of lower risk carcinogens. For noncarcinogens, weighting factors are not developed; rather, chemicals are categorized into two groups, high risk and low risk. High risk noncarcinogens can be traded on a one-to-one basis with other high risk noncarcinogens and with carcinogens on a ten-to-one basis. Reductions in high-risk noncarcinogens can offset low risk noncarcinogens, but not vice versa.

To identify high-risk chemicals in both the carcinogen and noncarcinogen categories, OAQPS first gathered available health data on the chemicals. For carcinogens, potency data was taken from IRIS and from CERCLA Reportable Quantities. Weight-of-evidence classifications and CERCLA hazard ranking (low, medium, high) was also recorded. IRIS was also used to obtain data for noncarcinogens. IRIS was supplemented by RTECS, where IRIS data were not available.

After health data were gathered, OAQPS performed generic exposure modelling based on average meteorologic conditions. If the chemical concentration 500 meters from the source posed greater than $1 \times 10^{-4}$ risk, or if the concentration exceeded the reference dose (or the LOEL/100 or LD50/1000, if no RfD was available) by an order of magnitude or more, the chemical was preliminarily designated "high-risk". The weighting factors for carcinogens were determined based on the ratio of the potency estimates of the high-risk chemicals to the potency estimates of the lower risk chemicals. In contrast, noncarcinogens were simply placed into high and low risk groups, without specific weighting factors. The last step in the analysis was to determine if any U.S. facilities actually emit these chemicals in sufficient quantities to reach the health effects benchmark of concern. This determination was based on TRI emissions data and other sources of emissions data. If at least one facility released the chemical in sufficient quantities to reach the benchmark exposure level. the chemical was included on the final "high-risk" list. Note that these emissions standards will be published in the Federal Register.

Pros: The relevant aspect of this proposal is the identification of chemicals that will count toward early emission reduction goals. Importantly, chemicals are ranked as high or low risk using generic air exposure modelling; this would support our use of such a generic approach. Secondly, the system implicitly ranks carcinogens against noncarcinogens by allowing weighted trading among the tow types of chemicals. The relative emission trading amounts would support a cancer versus noncancer severity weighting. The approach will be published in the Federal Register.

Cons: System considers only air emissions. System is tailored to a particular requirement of The Clean Air Act Amendments. The system does not address ecological effects.

## F. Other Agency Scoring and Ranking Systems

### 1. USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems

USEPA 1987, Prepared for the Administrator by
Richard Morgenstern, Director, Office of Policy Analysis
Don Clay, Deputy Assistant Administrator for Air and Radiation
Gerald Emison, Director, Office of Air Quality Planning and Standards
Rebecca Hanmer, Deputy Assistant, Administrator for Water
Marcia Williams, Director, Office of Solid Waste
PB88-127048, February 1987

This EPA report assesses 31 prominent environmental problems currently facing the United States. It attempts to rank them by the risk each poses to society in an effort to prioritize how EPA should use its resources. The environmental problems were defined along existing program lines, e.g. criteria air pollutants, hazardous air pollutants, contaminants in drinking water, Superfund sites, pesticide residues on food, worker exposure to toxic chemicals, etc. The ranking system that the authors employed has been published and peer reviewed by the Scientific Advisory Board.

Four different types of risks were evaluated for each environmental problem: cancer risks, non-cancer health risks, ecological effects, and welfare effects (visible impairment, materials damage, etc.). These risk evaluations did not consider the economic or technical controllability of the risks or the benefits to society of the activities causing the environmental problems. No attempt was made to combine the risk evaluations, so in effect four separate rankings of the 31 problems were generated.

The risk assessments were based on pollutant exposure and effects data. However, because the data were largely incomplete and the methodologies for evaluating them are undeveloped or crude, assessments were ultimately based on the collective informed judgement of the experts involved. Wherever possible, these judgements were made using formal and systematic methods.

## Cancer Risk

To assess carcinogenic risk, EPA relied on the Carcinogen Assessment Group's evaluation of the magnitude of risk. However, final rankings were based on judgment of the weight of evidence as well as magnitude.

## Non-Cancer Health Risk Evaluation

Each environmental problem was ranked based on the incidence of effects of the chemicals associated with each problem and weighted by the severity of the effects. The methodology began by selecting a few representative chemicals, for which incidence of exposure was estimated:

Incidence = number of people exposed X chemical potency
(potency = exposure dose divided by reference dose)

Data was often unavailable, in which case the authors' judgement was used. Incidences were summed, weighted by an effect severity index. The final rank was determined by scaling the sum by the authors' estimate of how much of the problem was not captured by the representative chemicals.

## Ecological Risk

The authors attempted a broad assessment of environmental impacts on all kinds of ecosystems from terrestrial and freshwater types to marine and estuarine types. However, their assessment was the least rigorous of the four. Each environmental problem was ranked by subjective consensus as high, medium or low for each type of ecosystem. The rankings were based on expert judgement of 1) potential anthrogenic impact on the environment at the local, regional and biospheric levels and, 2) the severity of the impact in terms of number of years required for ecosystem recovery once the stress was removed.

The judgements for a particular environmental problem were systematically aggregated across ecosystems to generate a high, medium or low overall ranking for the problem. However, the authors felt that their method was too inexact to try to establish relative rankings within these categories.

## Welfare Risk

A full range of welfare effects were considered, including soiling and other material damages, recreation, natural resources, damages to other public and commercial property and ground water supplies, and losses in aesthetics and non-user values. The environmental problems were ranked by consensus through a subjective review of the extent and cost of existing and potential damage.

Pros: Method is simple. Incorporates four broad risks/effects categories, being cancer risks, non-cancer risks, ecological effects, and welfare effects. These categories allow and require professional judgment in score determination. The cancer risk score uses both magnitude of risk as well as the weight of evidence. The non-cancer risk score uses exposure as well as severity of effect. This system has been published and reviewed by the Scientific Advisory Board.

Cons: The four different categories cannot be combined into a unified score. The professional judgment went into the score determination rather than the data selection, a process which would prove too unwieldy for the entire TRI database. Both the ecological and welfare ranks were subjective and relied upon site-by-site judgment rather than a rigorous method for calculation.

2. Integrated Environment Management Program

USEPA 1986, Prepared for the Environmental Criteria and Assessment Office, March

The IEMP is one system which seeks to incorporate the severity of the toxicity effect into a chemical release ranking system. The ranking of the chemical release is based upon its relative risk index score, calculated as:

RRIS = (Dose) * (Est. Potency for Human Health Effect) * (Weighting Factor)

Though the algorithm for determining the dose is not specified, the calculation is based upon: (1) pollutant loadings; (2) an exposure analysis using established Agency fate and transport models; (3) the population base identified; and (4) assumptions about body weight and routes of uptake.

Human health effects are divided into eight different categories, i.e. carcinogenicity, mutagenicity, etc.The health score is a function of the probability that the effect occurs in humans (T - based upon a set of decision rules regarding weight of evidence) and the probability of occurrence of the toxic effect (P). For carcinogens, P equals the risk per unit dose. For non-carcinogens,

$P = I/MED$

where I is the observed incidence of effects above the control incidence at the minimum effective dose (MED) expressed as (mg/kg/day).

The weighting factor is actually a severity factor for each toxic effect. They are intended to reflect the significance of the quality of life lost, years of life lost, and economic cost of the disease.

To the best of our knowledge, this system has been used only within the EPA and has not been publicly reviewed.

Pros: Method is simple. It uses both exposure and routes of exposure in its dose calculation. It incorporates eight different health effects in its health score and relies upon the weight of evidence. It can use one or all of these effects, allowing for gaps in the data. It contains a weighting factor for the severity of effect. It also generates a single score for carcinogens and non-carcinogens.

Cons: The system has not, to our knowledge, been peer reviewed. The specifics of the determination of the dose score and health score are not specified in the literature. The allowance of one to all of the health effects in the scoring makes a "fair" comparison among chemicals uncertain.

**3. Examination of the Severity of Toxic Effects and Recommendation of a Systematic Approach to Rank Adverse Effects**

USEPA 1986, Prepared for the Environmental Criteria and Assessment Office, March

Although this paper did not present a scoring system, it presents information on one aspect of scoring: the weighting of severity among different types of health noncancer effects. Note that it is an internal EPA document and has not undergone public review. The purpose of this paper is to differentiate the effects of chemicals upon the human body and then to rank those effects. For example, two different chemicals may have identical LOELs (Lowest Observable Effect Level) but that the "effects" may be entirely different, i.e. slight changes in the liver versus kidney and/or heart failure. Thus, while current research focusses on comparing chemicals according to these quantities, the author believes in the necessity of a simultaneous ranking system based upon both the type and magnitude of different toxic effects. This paper presents two ranking systems, one for histopathological lesions (direct physical impact upon organs) and one for biochemical effects.

The histopathological scheme lists the severity of effect as a function of the severity of the lesion, modified by any additional non-histopathological effects, and the affected organ. The expression for the severity score is:

Score = ((Lesion Severity) + (Non-hist. Modifier)) * Organ Factor

The lesion severity is determined from a table which lists eight possible ranges of effects and then assigns a score from one to eight (eight being the most severe) for that range. The modifier is simply an addend for three different non-histopathological effects: organ weight change, biochemical change, and organ system impairment. For an observed effect in each category, the modifier is one. For no observable effect, the modifier is zero. If it is unknown whether these effects accompany the lesion, the modifier is one-half. A

value is assigned to the organ factor according to a table which ranks each of the four "Organ Categories" defined in the report.

The algorithm for the endpoint toxicity scheme is similar. The severity score may be expressed as:

Score = ((Endpoint Severity) + (Endpoint Modifier)) * Organ Factor

The endpoint severity is determined from a table which lists seven possible ranges for the biochemical change or system impairment as well as the category of the affected organ. The table assigns a score, from one to seven, for each range, with seven being the most severe. The modifier, as in the first scheme, is equal to one, zero, or one-half, depending upon an observed, non-observed, or uncertain accompanying histopathological lesion or organ weight change. For example, a body weight change in an organism receives a score of one, the absence of organ weight change and lesions creates a modifier of zero for both and therefore a total modifier of zero. No effect in category one organs (lung, heart, brain, etc.) is an organ factor of one, yielding a total score of one.

The author cautions that these proposed schemes are not suitable for use in the comparison of chemicals because, since factors such as duration of exposure and route of exposure were not variables in the derivation of the schemes, these would need to be held as fixed in comparing chemicals, a situation which never occurs in toxic releases.

Pros: A relatively simple method. It examines the differences in the severity of effects. It includes rankings according to the organs affected, biochemical effects, and histopathological effects.

Cons: This is not an overall scoring system. The author even cautions against its integration into a scoring system because certain site-specific variables, such as duration or route of exposure, were not incorporated into the scheme. This system has not been peer reviewed.

In developing this severity ranking scheme, the authors of this paper reviewed several other systems that use severity as a factor in the comparison of chemicals. The following describes systems used by the author to develop their scoring systems.

**Assessment of Air Emissions from Hazardous Waste Treatment, Storage, and Disposal Facilities**

One hundred of the 501 RCRA wastes handled by treatment, storage, and disposal facilities (TSDFs) were ranked according to two types of health data, toxic effects and carcinogenic effects. Two factors were created, the toxicity hazard factor and the carcinogenicity hazard factor. These are described as:

THF = (gas-phase equil. conc.) / (Threshold Limit Value)
CHF = (gas-phase equil. conc.) / (max allow. conc. at the 1E-5 Risk Level)

The maximum allowable concentration at the 100,000 risk level is the concentration at which there is a 95% confidence that the limit on the cancer risk is one in one hundred thousand people. Each of these factors is then multiplied by the wastes' aqueous and nonaqueous disposal volumes in order to generate volume-weighted hazard scores.

In addition to the determination of these factors, a weighting factor is created from carcinogenicity, teratogenicity, and acute toxic effects of each contaminant (using data from RTECS). The score for each lies between zero and three. This weighting factor was then multiplied by the scores.

Pros: Simple system. Incorporates two different health effects, toxic effects and carcinogenic effects. It uses the volume of release directly in the score determination. Includes a weighting factor based upon carcinogenicity, teratogenicity, and acute toxic effects.

Cons: The two scoring factors for toxic and carcinogenic effects cannot be combined. The factors rely upon the Threshold Limit Value and the Maximum Allowable Concentration at the 1E-5 Risk Level respectively, data which exists for few chemicals. Does not have an exposure component.

**RCRA Risk-Cost Analysis Model:**

This model follows a five-step process in order to determine human health risks resulting from releases of chemicals. After chemical selection, concentrations of the contaminants are estimated for three transport processes (air, surface water, and groundwater). The model then estimates the total human intake, calculates the risk to an individual, and then estimates the population risk by multiplying by the total population in a given area. This process assigns a risk score which then ranks the releases.

Two equations were developed in order to model the process. They are:

Carc. Risk = (risk per unit dose)*(severity index)*(dose)^shape*(population exposed)
Non-Carc. Risk = (risk per unit dose)*(dose)*(population exposed)

The severity index follows from a 1984 EPA ranking system developed to quantify statutory reportable quantities of hazardous substances. It assigns a value of 0.1 for severities 1-2, 0.5 for 3-7, and 1.0 for 8-10. The shape is merely an exponent to determine the shape of the curve.

Pros: Simple System, requiring only a dose for mammalian species based upon either human or animal chronic or acute doses. Considers three different routes of exposure, oral, inhalation, and dermal.

Cons: Relies upon a narrow range of health effects. Does not have an exposure or a volume component (it ranks chemicals, not releases). Though the score only requires the dose, the calculation of the dose is a cumbersome and difficult to understand process.

**Toxicity Scoring System Using RTECS Data Bases:**

Though the scoring algorithm is simple, requiring only a dose, the methodology requires detailed toxicity data for input into the algorithm.

The only dose considered are those for mammalian species. This method only considers oral, inhalation and dermal routes of exposure, assuming each of equal importance and the absorption to be 100%. Four subscores are considered for each substance: human acute, animal acute, human chronic, and animal chronic. The final score is taken from the following hierarchy:

--> minimum of human and animal chronic doses, if both have entries;
--> chronic dose for humans or animals, if only one has entry;
--> minimum of human and animal acute doses, if both have an entry and there are no chronic entries; and
--> acute dose for humans or animals, if this is the only category with any entries

In using RTECS, chronic exposures are those resulting in effects other than death or are effects such as cancer which may result in mortality. Selecting a human chronic effect requires comparison in the RTECS data bases, where carcinogenic effects are classified as a carcinogenic response(CAR), a neoplastic response(NEO), or an equivocal tumorigenic agent(ETA). The lowest effect level for carcinogenicity is chosen by selecting the lowest dose of CAR or NEO. If neither exists, the lowest ETA is multiplied by two. The selected dose is modified when there are multiple carcinogenicity entries by decreasing the selected dose 10 percent per additional positive result, to a maximum of 50%. Teratogenic doses

from individual studies are ranked and the dose at the 20th percentile is selected as the teratogenic dose. This dose is lowered in the same manner as the carcinogenic dose.

Pros: Simple system. Incorporates exposure data for three different routes, air, surface water, and groundwater. It also incorporates the severity of effect according to a 1984 EPA ranking system, making its inclusion simple and straightforward.

Cons: Relies strictly upon the cancer slope of a chemical, limiting the number of allowable chemicals by available data. The two separate scores calculated, carcinogenic and non-carcinogenic, may not be compared.

## II. Survey of TRI Ranking and Indexing Efforts Outside EPA

A number of organizations outside of the Agency have also developed ranking/scoring systems for their own purposes, such as targeting chemicals for state regulation; identifying chemicals for poilution prevention projects; and assessing the hazard of TRI emissions in particular communities.

Abt Associates contacted a number of organizations which have utilized TRI data in publications. The organizations were asked about the scope and methodology used in their reports.

Rhone-Poulenc in Paris developed an Environmental Index (EI) to access the aqueous effluent impact of wastes. They computed a raw indicator as a weighted average of the daily mass of six types of wastes (toxic materials, suspended solids, nitrogen, phosphorus, salts, and chemical organics). No justification is given for these weights. The raw indicator is multiplied by 100 and divided by the average from the prior year to arrive at the final EI for the month. This transformation is intended to make comparisons easy. If the index is greater than 100 the impact has been greater, values less that 100 indicate improvement. (Rhone-Poulenc memo July 25, 1991)

Chemicals on Which Data Are Currently Inadequate: Selection Criteria for Health and Environmental Purposes

Organisation for Economic Co-operation and Development, Berlin, March 1985

This report itself did not present a chemical ranking system. Rather, the purpose of this task was to develop a rational methodology by which countries could select chemicals that most urgently need attention. The elements of this methodology were: identifying selection elements, exploring ways of weighting and combining elements and reviewing data sources. Selection elements identified included workplace exposure, general population exposure, environmental exposure, human and environmental effects. OECD also included recommendations for applying these elements. Importantly, OECD emphasized the importance of clarifying the purpose and scope of the selection exercise in order to define limits and interpretations. OECD also supported the use of expert judgment to fill in data

gaps. Finally, OECD strongly urged consideration of data quality in the ranking and selection of chemicals.

For each of the elements of the methodology, OECD broke the approach down into four steps: compilation, screening, refinement and review. The report then suggested topics to consider in each of the four phases.

Polaroid Corporation has developed a 5-category scheme for all chemicals that they use. Chemicals in categories i and ii are highly toxic (known and possible carcinogens). Category V chemicals are non-toxic solid waste. Chemical categories have been used to establish goals for 50 percent reduction in chemical use by category. The focus on chemical use reduction rather than chemical release reduction is based on the Massachusetts Toxics Use Reduction Act. Category specific goals are designed to prevent strategies that claim a "50 percent use reduction" but are based exclusively on reductions in use of low toxicity wastes. (Conversation with Polaroid Corporation representatives, June 1991)

The Boston Herald published a series of articles under the heading of "Ill wind," covering environmental releases of toxic chemicals in Massachusetts. The Herald concentrated mostly upon volumetric data but also developed an algorithm for ranking the chemical releases according to volume and toxicity. The algorithm multiplied the volume of release by a decimal number derived from the inhalation risk number. This enabled the article to rank individual emitters by order of "cancer risk." The Herald acknowledged that the ranking did not incorporate human exposure into its calculation and cautioned against using their calculation as an "actual measurement of risk"
(The Boston Herald, Monday, May 13, 1991, p. 8).

Air Toxic "Hot Spots" Program Risk Assessment Guidelines
California Air Pollution Control Officers Association, March 1990

This system is designed to prioritize facilities in accordance with the Air Toxics "Hot Spots" Information and Assessment Act of 1987. According to this act, any facility which qualifies as a "high priority" facility must perform a health risk assessment. Localities determine the priority level (high, intermediate, or low) of the facilities in their district based upon the facility's reported emissions of one or more of some 500 chemicals. Separate calculations and priority levels are used for carcinogenic and noncarcinogenic substances. The higher of the two levels as calculated is assigned to the facility.

The score for a facility emitting carcinogens is equal to the sum of the scores generated for each carcinogen. Each contaminant's score is calculated as

$$TS = \text{emissions [lbs/yr]} * \text{unit risk [ug/m}^3\text{]}^{-1} * \text{distance factor} * \text{normalization factor}$$

The distance factor is determined from the distance from the source of the emissions to the nearest populated area. That quantity corresponds to a value relating the change in

concentration with distance through the use of a Gaussian plume dispersion model. A total score of ten roughly corresponds to a risk of one in ten thousand and a total score of one similarly corresponds to a risk of one in one hundred thousand. This methodology places any facility scoring above ten in the "high priority" category and those scoring below one in the "low priority" category. A score between one and ten requires further analysis.

The score for a facility emitting non-carcinogens is determined much in the same way. The total score for the facility is the sum of the scores of each substance emitted by the facility. The substance score may be expressed as:

TS = emissions [lbs/yr[1]] * distance factor * normalization/acceptable exposure level [ug/m$^3$]

The non-carcinogenic scores are considered identically to the carcinogenic scores, with "high priority" assignment to facilities with totals over ten and "low priority" assignment to facilities with total scores below one. Note that the carcinogenic and non-carcinogenic scores are not added together.

**Louisiana's Environmental Action Plan "Leap to 2000"**

Public Advisory and Steering Committee Risk Ranking Retreat Briefing Material
March 26, 1991

Louisiana formed a Political Advisory Committee (PAC) to rank 33 environmental issues by the severity of risks they posed to the State. Risks were divided into three categories, human health, ecological effects, and quality of life. The issues were ranked separately within each of these categories based upon available scientific information and the judgement of assembled experts. Informed by the three rankings, the PAC settled the final comprehensive risk ranking by voting on the issues.

**Health Effects**

This method estimates risk to human health from the cancer and non-cancer effects. Cancer risk was calculated based on chemicals representative of each issue:

Risk = Environmental Concentration X Potency X Population Exposed

Thus the issues were ranked by estimated cancer cases that would be caused by a particular environmental problem. The issues were categorized as high, medium or low based on breaks in the data of these results.

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[1] maximum lbs/yr for substances associated with acute toxicity and average lbs/yr for substances associated with chronic toxicity

Non-cancer health risk was estimated from chemicals representative of each issue. Three exposure pathways were considered: air inhalation, food and liquid ingestion, and skin adsorption. Risk presented by each issue was calculated for each applicable exposure scenario as:

Risk = Severity Index X Dose X Population Score

The severity index is a standard ordinal ranking of body organs affected by a chemical and the severity of those affects. Dose is an ordinal score based on ranges of RfD divided by average contaminant concentration in the population's environment. Population score is an ordinal rank of ranges of population sizes.

Non-cancer health risk for an issue is calculated as the average of the risks posed by each exposure pathway. Issues were again ranked high, medium or low based on breaks in the data of these results.

The final issue ranking placed equal weight on the cancer and non-cancer effects. The nine possible combinations of the elements of the two categories were assigned very high, high, medium high, medium and low ranks based on a committee consensus.

Ecological Effects

The ranking committee ranked the environmental issues based on the degree to which nine ecosystems were affected by each issue. Impacts on each of the nine ecosystems were evaluated on an issue by issue basis by examining how stressors associated with an issue impacted the stress indicators in an ecosystem. For example, for the Terrestrial Habitat Loss issue, stressors like industrial development and proposed road construction were rated on a scale of 0 to 10 for how they affect such stress indicators as Changes in Nutrient Cycling and Loss of Habitat. A stressor's score was the weighted average of ratings across stress indicators, the weights reflecting the committee's assessment of relative importance of the stress indicators. Stressor scores were averaged to determine the final rating of the importance of the issue to the particular ecosystem.

The rank of the issue was calculated as the weighted average of these ecosystem-specific ratings, the weights reflecting the committee's assessment of the value of each ecosystem. Breaks in the ranking figures determined how the issues were divided into five categories (very high through low.) Separately, committee members voted on the ecological importance of each issue using the same five categories and compared this ranking to the quantitative one. The four issues that were not placed in the same categories by the two systems were recategorized by consensus.

Quality of Life

This analysis attempted to rank the issues into high, medium and low categories based on the costs associated with damages not accounted for in the two other rankings. Among these costs are health care costs, recreation losses, materials damage and aesthetic losses. The issues were first ranked based on the dollar value estimates of costs as determined by various relevant economic studies. The issues were ranked again based on qualitative assessments of changes in quality of life using such measures as the number of people suffering damages, and the reversibility of those damages. Equal weight was given to the quantitative and qualitative rankings in determining the final ranking (again using the very high through low categories.)

Purposes of and Criteria for Development of Chemical Hazard Lists from Ten Domestic and International Organizations

USEPA 1985, Prepared for the Office of Pesticides and Toxic Substances, Economics and Technology Division, December 31

This report reviewed various systems by which different organizations have compiled lists of chemicals which they believe ought to be monitored. Each of these steps involved selecting criteria in order to determine their placement upon the list as well as ranges. The following summarizes the findings of this report:

The European Communities Council Directive Chemical Hazard List:
82/501/EEC, OJ No L 230, 5.3.82, pp. 1-18 (June 24, 1982)

The EC has mandated that any industry must list their use of any of the 178 chemicals upon this list. The chemicals on this list fall into two toxic categories, very toxic substances, other toxic substances. The qualifications for these categories are as follows:

| "Very Toxic" Substances | Other Toxic Substances |
|---|---|
| $LD_{50}$ (oral) < = 5; or<br>$LD_{50}$(cutaneous) < = 10; or<br>$LC_{50}$ (inhalation) < = 0.1<br><br>or<br><br>5< $LD_{50}$ (oral) < = 25; or<br>10 < $LD_{50}$ (cutaneous) < = 50; or<br>0.1 < $LC_{50}$ (inhalation) < = 0.1<br>and<br>Physical and chemical properties which cause effects similar to those caused by chemicals which fall into the above criteria | 25 < $LD_{50}$ (oral) < = 200; or<br>50 < $LD_{50}$ (cutaneous) < = 400; or<br>0.5 < $LC_{50}$ (inhalation) < = 2 |

**California Air Resource Board Toxic Chemical List & NIOSH/OSHA Pocket Guide:**
Air Resources Board of the State of California

The NIOSH/OSHA Pocket Guide to Chemical Hazards is a list of 380 chemicals, all under federal regulation, which includes information on and recommendations concerning each of these chemicals. The object of this list is to compile chemicals most likely to travel downwind in the event of an accidental release. The California Air Resources Board included on its list any chemical from the guide with an IDLH (Immediately Dangerous to Life and Health - maximum concentration of a substance from which one could escape within 30 minutes without any escape-impairing symptoms or any irreversible health effects) below 2000 ppm and a vapor pressure greater than 20 mmHg.

**New Jersey Department of Environmental Protection Highly Toxic Substances List:**
State of New Jersey Department of Environmental Protection, Division of Environmental Quality

The division of Environmental Quality in the Department of Environmental Protection in New Jersey sought to prepare a list of chemicals which would cause acute health effects if released into the air. Their toxicity criterion was based upon a Threshold Limit Value (TLV - time-weighted average concentration to which nearly all workers may be repeatedly exposed without adverse effect) of one pm. An additional criterion for inclusion on the list was reactivity. Volatility and usage were used to rank the chemicals. but the methodology is not included in the report.

**Department of Transportation Poisonous Substances List:**
DOT Hazardous Materials Regulations 49 CFR 172.101

The DOT's Hazardous Materials Table includes two categories for poisonous substances, Poison A and Poison B. Poison B materials meet the following requirements:

$LD_{50}$(oral) < = 50 mg/kg
$LC_{50}$ (inhalation) < = 2 mg/l (if such a conc. is likely)
$LD_{50}$ (cutaneous) < = 200 mg/kg

The Poison List has 153 chemicals of which 141 are Poison B materials.

**Philadelphia Air Pollution Control Board Toxic Air Contaminants List:**
Air Management Regulation VI: Control of Emissions of Toxic Air Contaminants, Air Pollution Control Board of the Philadelphia Department of Public Health, 1981

Two lists were developed in order to require emissions reports from industry. The criteria for the development of Schedule A are not specified, though the methodology incorporated risk of immediate harm, carcinogenicity, mutagenicity, tertogenicity, bioaccumulative effects, and whether the chemical is known to be present in the Philadelphia area. The criteria for schedule B are identical and also meet the definition of "pollutant" as established by the EPA. The two schedules encompass a total of 104 chemicals.

**Union Carbide Corp. Industrial Hygiene Sampling and Monitoring Program List**
Union Carbide Institute plant, 1984

Union Carbide developed a list of priority chemicals for their monitoring program at their plant in Institute, West Virginia. The chemicals have been ranked ordinally from one to four in the following system:

| Rating 4 | Rating 3 | Rating 2 | Rating 1 |
|---|---|---|---|
| Have OSHA, ACGIH, or UCC standards (whichever is lower) including permissible exposure limits (PEL) of less than 5 pm or less than 0.1 mg/m8 as TWA8 (time weighted average for normal 8 hr. day)<br><br>known carcinogens<br><br>result in mutagenesis, teratogenesis, or fertility impairment in humans<br><br>result in irreversible nerve damage<br><br>result in irreversible long-term organ toxicity<br><br>are fast-acting and can produce major injury | $5 < PEL < 25$ or $.11 < TWA_8 < 1.0$<br><br>supposed human carcinogens, mutagens and teratogens<br><br>result in hematologic disturbances<br><br>result in respiratory of skin sensitization<br><br>produce narcosis | $26 < PEL < 200$ or $1.1 < TWA_8 < 5$<br><br>produce severe irritation of the skin, eyes, or respiratory system<br><br>are anoxiants | $PEL > 200$ or $TWA_8 > 5$<br><br>classified as simple asphyxiants or nuisances<br><br>have generally low risk effects |

The ranking of the chemical determines how often they are to be sampled within the plant.

As can be noted, each of these systems represents a methodology for chemical selection and presents, at best, a simplistic means for ranking chemicals according to different properties. Nonetheless, it presents a large sample of properties (PEL, IDLH, etc.) which have been used in the differentiation of chemical toxicity.

**Other Systems**

Our research has uncovered three systems for which we are still trying to obtain documentation. They are an Office of Water TRI chemical ranking system, an EPA compound evaluation system, and the National Air Toxics Information Clearinghouse pollutant selection and prioritization method. We also found two systems that were not relevant to this TRI indicator discussion. The documents supporting these systems are titled 1) Existing Chemicals of Environmental Relevance (German Chemical Society, October 1985) and 2) Chemical Scoring System Development (Oak Ridge National Laboratory.)

# Appendix B

# Options for a TRI Indicator Ranking/Scoring System

## Appendix B

## OPTIONS FOR A TRI INDICATOR RANKING/SCORING SYSTEM


**I. Elements of a Scoring System** . . . . . B-3

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## I. Elements of a Scoring System

A separate memorandum summarizes a number of chemical scoring and ranking procedures used by Offices within the Agency and by organizations outside of the Agency. From the review of these scoring systems, several common issues emerge. These issues must be addressed in the development of a ranking system for the TRI index. These issues include:

a. Selecting measures on which the ranking will be based
   Choosing measures to describe a chemical's toxicity and potential exposure

b. Selecting a method to score the measures. Options include:
   Qualitative - high, medium or low
   Ordinal - 1, 2, 3
   Weighted - 10, 100, 1,000
   Calculated - continuous values

c. Selecting ranges over which measures are assigned scores
   For example, an RfD may be scored a 1 if it ranges from 5 to 0.5 and a 10 if it ranges from 0.5 to 0.05
   Weight-of-evidence categories might also be scored

d. Factoring data quality into the index

e. Using severity indices to weight chemical scores within a category

f. Ranking individual chemicals or forming sub-indices
   Each chemical is described by scores in a variety of categories (e.g. acute toxicity, neurotoxicity, cancer). If we establish the relative importance of risks among these categories, a chemical's scores can be combined across categories to form a chemical rank. We can also choose to not judge the relative importance of the risks. Instead, we can generate an indicator for each category.

g. Methods of establishing the relative importance of risks among categories
   Relative importance is reflected by the methodology used to combine a chemical's scores across categories. Various methods include simple summation, multiplication, other mathematical functions, matrices, taking the worst score, and establishing decision rules

h. Weighting scores: an alternative to methods presented in Section I.g.
   One alternative method to those presented in I.g.

The review of the scoring systems within and outside of the Agency has suggested a number of approaches for handling each of these issues. Several alternative approaches for each

issue, and their advantages and disadvantages, are described below.

a. Selecting measures on which the ranking will be based

Measures include all of the parameters that will be incorporated into the scoring system. Some will describe the toxicity and physicochemical properties of a chemical (e.g., $LD_{50}$, RfD, solubility), others will describe exposure at a site (e.g., volume of release, population, site environments.) A decision will need to be made concerning which chemical properties to incorporate into the scoring system. The Section 313 criteria lists ten parameters that EPA must consider when evaluating a chemical for addition to TRI: carcinogenicity, chronic toxicity, acute toxicity, reproductive toxicity, heritable gene and chromosomal mutations, developmental toxicity, neurotoxicity, environmental toxicity, persistence and bioaccumulation (these parameters are defined in Appendix A.) Most of the scoring systems we reviewed consider at least some of these categories, although they are frequently merged into fewer parameters. The categories should be chosen to reflect different risks posed by the chemicals so that a particular risk is not overstated by virtue of being represented in more than one category.

The index will also incorporate measures of potential exposure including media-specific emissions volumes, site characteristics and physicochemical properties. Site characteristics include the potential population exposed through different media, and factors such as stream volume and wind speed that influence the transport and dispersion of a chemical in the environment. Physicochemical properties typically include partitioning, dilution, and dispersion coefficients of contaminants.

b. Selecting a method to score the measures

Once measures for describing toxicity and exposure have been selected, a system for evaluating these measures must be chosen. The goal is to derive some way of scoring chemicals relative to one another within each category. Possible categories might be human carcinogenicity, human chronic toxicity, mammalian acute toxicity, chronic toxicity for aquatic species, and physicochemical exposure potential.

One system uses qualitative divisions to score chemicals within a category. For example, the carcinogenicity of a chemical might be scored "high", "medium", or "low." An advantage to using qualitative scores is that structure activity relationships can be used to assign scores to chemicals without specific toxicity or exposure data. A disadvantage of qualitative scores is that they only broadly distinguish toxicity and exposure potentials and do not allow for more refined consideration of potency or exposure factors. Thus, two carcinogens such as benzene ($q_1^*$ = 0.029) and dieldrin ($q_1^*$ = 20) could both be scored "high," despite the fact that they have very different potencies.

Ordinal systems (e.g. 1, 2, or 3) group chemicals in a similar fashion. Note that ranking formulas that incorporate ordinal scores should not be used to attribute proportional meaning to the ordinal scores. Because assigning an ordinal rank of 3 to chemical A and 1 to chemical B

does not mean chemical A is three times worse than chemical B, mathematical functions involving these two scores only convey information on order, not on proportional magnitude.

Unlike ordinal systems, weighted scoring systems (e.g. 1, 10, 100, 200) use numerical scores that reflect the proportional differences between chemicals. For example, within a category like physicochemical exposure potential, weighted scores could reflect the proportional magnitudes of volatility among chemicals.

Another way to score chemicals within a category is to use the actual value of a measure or mathematical function of the measure. For example, carcinogenicity might be scored by using the actual $q_1^*$ of each chemical. Unlike systems that assign scores to categories of chemicals (e.g., low, medium, high) and thus do not differentiate between chemicals with the similar properties, this kind of system compares chemicals on a continuous scale.

Unfortunately, rankings based upon more specific scores (based on $q_1^*$ or on chemical-specific decay rates, for example) require data that is available for only a limited number of chemicals, thereby restricting the number of chemicals that could be considered in the index. When specific values are not available, other scores that consider relative potency in a general way (such as RQ values) can be used. Adjusted RQs consider exposure potential as well by adjusting the toxicity score by a degradation factor based on biodegradation, hydrolysis and photolysis (BHP). Using RQs would allow us to take advantage of work that the Agency has already done to categorize and score chemicals based on toxicity and exposure considerations.

More refined exposure scores can be obtained using simplified exposure modelling. One measure is site-specific population-weighted contaminant concentration. Concentration can be estimated using physicochemical properties such as solubility coefficients and environmental site characteristics like stream flow rates and distances to drinking water uptakes. Population densities are used to weight contaminant concentrations. Typically, scoring is often done separately for different exposure pathways and a chemical often scores very differently depending on the pathway (e.g., low for drinking water, high for fish consumption.)

c. Selecting ranges over which measures are assigned scores

If a scoring system is used to rank chemicals within a category, each score must be assigned to a range of values of the underlying measure. For example, the 307(a) Priority Pollutants Chemical Ranking methodology used the following ranges to score the aquatic toxicity of chemicals:

| Score | $LC_{50}$ (mg/L) |
|---|---|
| 12 | < 0.1 |
| 10 | 0.1 - 1.0 |
| 5 | 1.0 - 10.0 |
| 3 | 10.0 - 100 |
| 0 | > 100 |

Other types of data used to determine the cutoffs include RfDs (non-carcinogens) and $q_1^*$ (carcinogens), RQs (or TPQs where RQs not available), and occupational levels.[1] The selection of ranges forces a tradeoff between 1) using a large number of narrow ranges, which might imply that the data is more refined than it really is, and 2) using a small number of broad ranges which inflates or diminishes the importance of the boundaries and the measures that fall near them.

More than one kind measure can be used to score chemicals within a category. This approach takes advantage of a broader data set to score chemicals, including structure activity relationships. For example, for acute mammalian toxicity, we may have several kinds of toxicity data that describe a chemical's potency, such as acute oral $LD_{50}$ and acute dermal $LD_{50}$. If only one measure were available, it would be used to determine the chemical's rank in that category. If both were available, the more restrictive value could be used. Alternatively, we could create a hierarchy of preferred measures; in this case, we may prefer to use oral toxicity over dermal toxicity for the drinking water exposure pathway, where both are available. The advantages of this method are that data gaps are minimized.

The selection measures, boundaries for scoring measure ranges, and category scores are presented in Tables 1, 2, 3 and 4 for selected scoring systems reviewed in this memo. Our review demonstrates that vast effort and expertise has already been devoted to scoring and categorizing chemicals, both within the Agency and externally. This expertise could be built upon in the development of the TRI index.

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[1] Edward J. Calabrese and Elaina M. Kenyon, "The Perils of State Air Toxic Programs," *Environmental Science and Technology*, Vol. 23, No. 11 (November 1989), 1326-9. This article warns against using occupational levels for general population risk screening, for several reasons: (a) occupational levels consider a recovery period between exposures; (b) occupational levels consider the "healthy worker" effect (that is, the levels are set for protection of relatively healthy populations), (c) the ACGIH levels are set based on data of unknown quality (d) the levels do not account for environmental fate (persistence, bioconcentration) and multiple exposure sources.

# Table 1: Human Toxicity Parameter Ranges

<table>
<tr><th>Ranking Systems</th><th>Human Acute Toxicity</th><th>Human Chronic Toxicity</th></tr>
<tr><td>Screening Methodology for Pollution Prevention Targeting<br>(USEPA, date unknown, prepared for OTS)</td><td></td><td>Carcinogenicity:<br>high = 3<br>med = 2<br>low = 1<br><br>all B2 carc. given a score of 3<br><br>Neuro:<br>high = 3<br>med = 2<br>low = 1<br><br>Developmental:<br>high = 3<br>med = 2<br>low = 1</td></tr>
<tr><td>TSCA Chemical Scoring System for Hazard and Exposure Identification (O'Bryan, T. R. and Ross, R. H. 1988, Journal of Toxicology and Environmental Health, Vol (1):119-134)</td><td>
<table>
<tr><th>Inhalation LC50</th><th>Dermal LD50</th><th>Oral LD50</th><th>Exposure Level</th><th>Score</th></tr>
<tr><td>< 50 mg/m3</td><td>200 mg/k</td><td>< 50 mg/kg</td><td>Low</td><td>7-9</td></tr>
<tr><td>50-500</td><td>200-500</td><td>50-500</td><td>Medium</td><td>4-6</td></tr>
<tr><td>> 500</td><td>> 500</td><td>> 500</td><td>High</td><td>1-3</td></tr>
</table>
</td><td>
Score Genotoxicity:<br>
9 Evidence of mammalian mutagenicity/clastogenicity, interaction with mammalian germ cell DNA, or epidemiological data suggesting genotoxicity in humans<br>
8 Evidence of genotoxicity in non-mammalian germ cell assays, or evidence of mammalian dominant lethality<br>
5-7 Evidence of genotoxicity in more than one test system, other than above<br>
2-4 Limited evidence of genotoxicity, including mixed positive and negative results<br>
1 Limited evidence of nongenotoxicity<br>
0 Negative test results indicating lack of known genotoxicity<br><br>
Score Carcinogenicity:<br>
8-9 Evidence of oncogenicity from epidemiological studies or positive results in two or more mammalian species<br>
6-7 Evidence of oncogenicity in either sex of a single mammalian species<br>
4-5 Suggestive evidence of oncogenic potential from epidemiological studies, mammalian bioassays, cell transformation in vitro, or promoter/carcinogenic activity<br>
3 Evidence of genotoxic potential<br>
1-2 Limited evidence of lack of oncogenic potential<br>
0 No evidence of oncogenic potential from well-conducted and well-designed mammalian studies in two or more animal species
</td></tr>
</table>

# Table 1: Human Toxicity Parameter Ranges

| Ranking Systems | Human Acute Toxicity | Human Chronic Toxicity |
|---|---|---|
| TSCA Chemical Scoring System for Hazard and Exposure Identification (concluded) | | Score *Developmental Effects:*<br>8-9 Evidence of adverse developmental effects in humans or at least two other mammalian species<br>6-7 Evidence of adverse developmental effects in one mammalian species<br>5 Developmental effets at doses accompanied by maternal toxicity or otherwise equivocal test results<br>4 Adverse developmental effects in nonmammalian species or in vitro test systems<br>3 Indirect evidence suggesting possilbe adverse developmental effects<br>2 Indirect evidence of lack of adverse developmental effects<br>1 Limited evidence of lack of developmental effects<br>0 No evidence of developmental toxicity potential |
| Toxic Chemical Release Inventory Risk Screening Guide (USEPA 1989, prepared by the Office of Toxic Substances, Volume 1, July) | Acute RQ / Ranking<br><= 100 lbs / Group 1<br>1,000 / Group 2<br>5,000 / Group 3 | Inhalation or Oral Rfd / Q1* / Cancer or chronic RQ / TPQ / Ranking<br><0.01 mg/kg-day / All / <= 100 lbs / = 100 lb / Group 1<br>0.01-0.1 / 1,000 / 500 / Group 2<br>>=1.0 / 5,000 / >= 1,000 / Group 3 |
| Ranking the Relative Hazards of Industrial Discharges to POTWs and Surface Waters (USEPA 1991, prepared for OPA, February) | | *Carcinogenicity:* Cancer RQ Value Used Directly<br>*Non-cancer chronic:* Chronic RQ Value Used Directly |

# Table 1: Human Toxicity Parameter Ranges

<table>
<tr><th>Ranking Systems</th><th>Human Acute Toxicity</th><th>Human Chronic Toxicity</th></tr>
<tr>
<td>Hazard Ranking System:<br>Final Rule<br>(55 Federal Register No. 241,<br>pp. 51532-667, 12/14/90)</td>
<td>
<table>
<tr><th>LD50<br>(oral)</th><th>LD50<br>(dermal)</th><th>Ranking:</th></tr>
<tr><td>< 5 mg/kg</td><td>< 2 mg/kg</td><td>1,000</td></tr>
<tr><td>5-50</td><td>2-20</td><td>100</td></tr>
<tr><td>50-500</td><td>20-200</td><td>10</td></tr>
<tr><td>> 500</td><td>> 200</td><td>1</td></tr>
<tr><td>not available</td><td>not available</td><td>0</td></tr>
</table>
<table>
<tr><th>LC50<br>(dust or mist)</th><th>LC50<br>(gas or vapor)</th><th>Ranking:</th></tr>
<tr><td>< 0.2 mg/l</td><td>< 20 mg/l</td><td>1,000</td></tr>
<tr><td>0 2-2</td><td>20-200</td><td>100</td></tr>
<tr><td>2-20</td><td>200-2,000</td><td>10</td></tr>
<tr><td>> 20</td><td>> 2,000</td><td>1</td></tr>
<tr><td>not available</td><td>not available</td><td>0</td></tr>
</table>
</td>
<td>
Carcinogenicity:
<table>
<tr><th>Class A,<br>Slope Factor</th><th>Class B,<br>Slope Factor</th><th>Class C,<br>Slope Factor</th><th>Ranking:</th></tr>
<tr><td>0.5 <</td><td>5 <</td><td>50 <</td><td>10,000</td></tr>
<tr><td>0.05-0.5</td><td>0 5-5</td><td>5-50</td><td>1,000</td></tr>
<tr><td>< 0.05</td><td>0.05-0.5</td><td>0.5-5</td><td>100</td></tr>
<tr><td>-</td><td>< 0.05</td><td>< 0 5</td><td>10</td></tr>
<tr><td>not available</td><td>not available</td><td>not available</td><td>0</td></tr>
</table>
Non-cancer chronic:
<table>
<tr><th>RfD<br><0.0005 mg/kg/day</th><th>Ranking:</th></tr>
<tr><td>0.0005-0.005</td><td>10,000</td></tr>
<tr><td>0.005-0.05</td><td>1,000</td></tr>
<tr><td>0.05-0.5</td><td>100</td></tr>
<tr><td>0.5 <</td><td>10</td></tr>
<tr><td>not available</td><td>1</td></tr>
<tr><td></td><td>0</td></tr>
</table>
</td>
</tr>
<tr>
<td>A Ranking System for Clean<br>Water Act Section 307(a) List<br>of Priority Pollutants<br>(USEPA 1985, July)</td>
<td></td>
<td>
<table>
<tr><th>Score</th><th>Carcinogenicity:</th></tr>
<tr><td>12</td><td>Proven human carcinogen</td></tr>
<tr><td>10</td><td>Potential human carcinogen, proven animal carcinogen</td></tr>
<tr><td>5</td><td>Potential animal carcinogen, proven mutagen, proven teratogen</td></tr>
<tr><td>2</td><td>Potential mutagen, potential teratogen</td></tr>
<tr><td>0</td><td>No carcinogenic, mutagenic, or teratogenic properties</td></tr>
</table>
</td>
</tr>
</table>

# Table 1: Human Toxicity Parameter Ranges

| Ranking Systems | Human Acute Toxicity | Human Chronic Toxicity |
|---|---|---|
| USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems (USEPA 1987, prepared by OPA, OAR, OAQPS, OW, and OSW, February) | | Dose/RfD: 1-10 → Score 1; 10-100 → 2; 100-1,000 → 3; > 1,000 → 4 |
| Assessment of Air Emissions from Hazardous Waste Treatment, Storage, and Disposal Facilities, (USEPA 1986) | | Threshold Limit Value (TLV) Used Directly (Concentration Units) |
| Air Toxics "Hot Spots" Program Risk Assessment Guidelines (CAPCOA, March 1990) | | *Air:* *Carcinogenicity:* $q^*$ Used Directly; *Non-cancer chronic:* RfD Used Directly |
| Louisiana's Environmental Action Plan "Leap to 2000" (Public Advisory and Steering Committee Risk Ranking Retreat Briefing Material March 26, 1991) | | Dose/Rfd: 1-2 → Score 1; 2-10 → 2; 10-100 → 3; > 100 → 4 |

# Table 2: Environmental Toxicity Ranges

| Ranking Systems | Aquatic Toxicity | Ecotoxicity | Mammalian Toxicity |
|---|---|---|---|
| **TSCA Chemical Scoring System for Hazard and Exposure Identification (O'Bryan, T. R. and Ross, R. H. 1983, Journal of Toxicology and Environmental Health, Vol (1):119-134)**<br><br>Acute LC50 or EC50 / Life cycle or Chronic NOEL / Score<br>< 1 / < 0.1 / 8-9<br>1-10 / 0.1-1 / 6-7<br>10-100 / 1-10 / 4-5<br>100-1,000 / 10-100 / 1-3<br>> 1,000 / > 100 / 0 | | | |
| **Toxic Chemical Release Inventory Risk Screening Guide (USEPA 1989, prepared by the Office of Toxic Substances, Volume 1, July)**<br><br>WQC / Aquatic RQ / Ranking<br><= 100 lbs / <= 100 lbs / Group 1<br>500 / 1,000 / Group 2<br>>= 1,000 / 5,000 / Group 3 | | | TPQ / Ranking<br><= 100 lbs / Group 1<br>500 / Group 2<br>>= 1,000 / Group 3 |
| **Ranking the Relative Hazards of Industrial Discharges to POTWs and Surface Waters (USEPA 1991, prepared for OPA, February)**<br><br>RQ Used Directly | | | |
| **Hazard Ranking System; Final Rule (55 Federal Register No. 241, pp. 51532-667, 12/14/90)** | | *Surface Water:*<br><br>Acute AWQC or AALAC / Chronic AWQC or AALAC / Assigned Value<br>< 1 ug/l / < 100 ug/l / 10,000<br>1-10 / 100-1,000 / 1,000<br>10-100 / 1,000-10,000 / 100<br>100-1,000 / 10,000-100,000 / 10<br>> 1,000 / > 100,000 / 1 | |

# Table 3: Exposure Parameter Ranges

<table>
<tr><th>Ranking Systems</th><th>Exposure Potential</th><th>Exposure Level</th><th>Population Level</th></tr>
<tr>
<td>TSCA's TRI Chemical Risk Assessment Pre-Screening Methodology (USEPA, date unknown, memo from OTS)</td>
<td>none = no expected release</td>
<td>
Criteria / Score<br>
> 700 mg/yr / 3<br>
70 to 700 / 2<br>
< 70 / 1
</td>
<td>
Surface Water:<br>
Criteria / Score<br>
> 10E6 people / 3<br>
10E5-10E6 / 2<br>
< 10E5 / 1<br>
Ambient Air:<br>
Criteria / Score<br>
> 10E5 people / 3<br>
10E4-10E5 / 2<br>
< 10E4 / 1<br>
Ground Water:<br>
Criteria / Score<br>
> 25,000 people / 3<br>
5,000-25,000 / 2<br>
< 5,000 / 1
</td>
</tr>
<tr>
<td>TSCA Chemical Scoring System for Hazard and Exposure Identification (O'Bryan, T. R. and Ross, R. H. 1988, Journal of Toxicology and Environmental Health, Vol (1):119-134)</td>
<td>
Half-life / Score<br>
> 1 yr / 5<br>
8-52 wk / 4<br>
2-8 wk / 3<br>
1-14 days / 2<br>
< 1 day / 1<br><br>
BCF / Log P / Score<br>
> 1,000 / > 4.35 / 9<br>
200-1,000 / 3.5-4 35 / 7<br>
100-200 / 3 18-3.5 / 5<br>
10 100 / 2.0-3 18 / 3<br>
< 10 / < 2 0 / 0
</td>
<td></td>
<td></td>
</tr>
</table>

# Table 3: Exposure Parameter Ranges

| Ranking Systems | Exposure Potential | | | | | Exposure Level | Population Level |
|---|---|---|---|---|---|---|---|
| Toxic Chemical Release Inventory Risk Screening Guide (USEPA 1989, prepared by the Office of Toxic Substances, Volume 1, July) | Henry's Constant<br>> 10E-2 atm-m3/mol<br>< 10E-6 | Log Koc<br>< 1.5<br>> 4.5 | BCF<br>> 1,000<br>< 250 | Atmospheric Half-life<br>> 1 year<br>< 1/2 day | Ranking<br>High Concern<br>Low Concern | | |
| | Aquatic Half-lives<br>> 1 year | Air Degradation Rate<br>> months | Water Degradation Rate<br>> months | Rate of Removal in bio. treatment<br>Log Kow < 1.5<br>Hc < 10E-5<br>resistant to degr. | Ranking<br>High Concern | | |
| | < 1/2 day | 1-7 days | 1-7 days | rapidly removed:<br>-P for phys/chem<br>-B for biodegr. | Low Concern | | |
| Hazard Ranking System; Final Rule (55 Federal Register No. 241, pp. 51532-667, 12/14/90) | *Surface Water:* | | | | | | |
| | Half Life (Lakes)<br>< 0.02 days<br>0.02-2<br>2-20<br>> 20 | Half Life (Other)<br>< 0.2 days<br>0.2-0.5<br>0.5-1.5<br>> 1.5 | Log Kow<br>< 3.5<br>3.5-4<br>4-4.5<br>> 4.5 | Assigned Value<br>0.0007<br>0.07<br>0.4<br>1 | | | |

# Table 3: Exposure Parameter Ranges

<table>
<tr><th>Ranking Systems</th><th>Exposure Potential</th><th>Exposure Level</th><th>Population Level</th></tr>
<tr><td>Hazard Ranking System; Final Rule (concluded)</td><td>
Surface Water:<br><br>
Use priority: availablity of BCF, LogKow, water solubility<br><br>
<table>
<tr><th>Assigned Value</th><th>BCF</th><th>Log Kow</th><th>Water Solubility</th></tr>
<tr><td>50,000</td><td>> 10,000</td><td>5.5-6.0</td><td>< 25 mg/l</td></tr>
<tr><td>5,000</td><td>1,000-10,000</td><td>4.5-5.5</td><td>25-500</td></tr>
<tr><td>500</td><td>100-1,000</td><td>3.2-4.5</td><td>500-1,500</td></tr>
<tr><td>50</td><td>10-100</td><td>2.0-3.2</td><td>-</td></tr>
<tr><td>5</td><td>1-10</td><td>0.8-2.0</td><td>-</td></tr>
<tr><td>0.5</td><td>< 1</td><td>< 0.8</td><td>> 1,500</td></tr>
</table>
<br>
Air:<br><br>
<table>
<tr><th>Vapor Pressure</th><th>enry's Constan</th><th>Assigned Value</th></tr>
<tr><td>> 10 Torr</td><td>0.001 atm-m3/</td><td>3</td></tr>
<tr><td>10-0.001</td><td>10E-5 to 0.001</td><td>2</td></tr>
<tr><td>0.001-0.00001</td><td>10E-7 to 10E-5</td><td>1</td></tr>
<tr><td>< 0.00001</td><td>< 10E-7</td><td>0</td></tr>
</table>
<br>
Ground Water:<br><br>
<table>
<tr><th rowspan="2">Water Solubility</th><th colspan="4">Distribution Coefficient (Kd) (ml/g)</th></tr>
<tr><th>Karst</th><th>< 10</th><th>10-1,000</th><th>> 1,000</th></tr>
<tr><td>Liquid</td><td>1</td><td>1</td><td>0.01</td><td>0.0001</td></tr>
<tr><td>> 100 mg/l</td><td>1</td><td>1</td><td>0.01</td><td>0 0001</td></tr>
<tr><td>1-100</td><td>0.2</td><td>0.2</td><td>0.002</td><td>2.0E-05</td></tr>
<tr><td>0 01-1</td><td>0 002</td><td>0 002</td><td>2.0E-05</td><td>2.0E-07</td></tr>
<tr><td>< 0.01</td><td>2.0E-05</td><td>2 0E-05</td><td>2.0E-07</td><td>2 0E-09</td></tr>
</table>
</td><td></td><td></td></tr>
</table>

# Table 3: Exposure Parameter Ranges

| Ranking Systems | Exposure Potential | | | Exposure Level | Population Level |
|---|---|---|---|---|---|
| **A Ranking System for Clean Water Act Section 307(a) List of Priority Pollutants (USEPA 1985, July)** | **Half Life** | **Hydrolysis Rate** | **Score** | | |
| | > 12 mo | - | 8 | | |
| | 6-12 mo | - | 5 | | |
| | 3-6 mo | > 3 mo | 2 | | |
| | 48 hr - 3 mo | 48 hr - 3 mo | 0 | | |
| | 24-48 hr | < 48 hr | -5 | | |
| | < 24 hr | - | -8 | | |
| | **Henry's Constant** | **KD value** | **Score** | | |
| | < 10E-3 | < 0.01 | 2 | | |
| | 0.001-0.01 | 10E2-10E4 | 0 | | |
| | > 0.01 | > 10E4 | -5 | | |
| | **BAF** | **Log P** | **Score** | | |
| | < 4,000 | < 6 | 8 | | |
| | 700-4,000 | 4.5-6 | 5 | | |
| | 300-700 | 4-4.5 | 2 | | |
| | > 300 | >4 | 0 | | |
| **Screening Procedure for Chemicals of Importance to the Office of Water (USEPA 1986, prepared by OHEA, November)** | **For human and aquatic populations:** | | | | |
| | **BCF** | **Score** | | | |
| | > 1,000 | High | | | |
| | < 1,000 | Low | | | |
| **USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems (USEPA 1987, prepared by OPA, OAR, OAQPS, OW, and OSW, February)** | | | | | ***Non-Cancer Effects:*** **People Exposed** / **Score**: <1,000 / 1; 1,000-10E5 / 2; 10E5-10E7 / 3; > 10E7 / 4 |

# Table 3: Exposure Parameter Ranges

| Ranking Systems | Exposure Potential | Exposure Level | Population Level |
|---|---|---|---|
| Louisiana's Environmental Action Plan "Leap to 2000" (Public Advisory and Steering Committee Risk Ranking Retreat Briefing Material March 26, 1991) | | | Population Exposed / Score<br>1-400 / 1<br>400-4,000 / 2<br>4,000-40,000 / 3<br>40,000-400,000 / 4<br>> 400,000 / 5 |
| California Air Resource Board Toxic Chemical List & NIOSH/OSHA Pocket Guide (Air Resources Board of the State of California) | *Air:*<br>Dangerous:<br>IDLH < 2000 ppm<br>and<br>vapor pres. > 20 mmHg | | |

# Table 4: Severity of Effect Measures

| Ranking Systems | Severity of Effect |
|---|---|
| USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems (USEPA 1987, prepared by OPA, OAR, OAQPS, OW, and OSW, February) | *Ranking of Organs*<br><br>Category I<br>Includes organs, impairment or loss of which is fatal and cannot be compensated for at all, or only heroic measures (i.e. expensive mechanical devices, transplantation). Also includes gonads, loss of which prevents reproduction.<br>Lung, heart, brain/spinal cord, kidney, liver, bone marrow, gonads<br><br>Category II<br>Includes organs whose loss or impairment may be fatal, but which can be compensated for by replacement therapy. Also includes organs, impairment or loss of which indicates an adverse effect on immune function or hematopoietic function which may be life threatening.<br>Adrenal, thyroid, parathyroid, pituitary, pancreatic islets, pancreas, esophagus, stomach, small intes large intestine, lymph node, spleen, thymus, trachea, pharynx, urinary bladder, skin<br><br>Category III<br>Impairment or loss of any of these organs is not life threatening but may result in severe functional emotional handicaps.<br>Accessory reproductive organs (oviduct, epididymis, uterus, prostate, coagulating gland, seminal vesical, ductus deferens, penis, vagina), eye, bone, nose, nerve, muscle, urinary bladder, blood ves ear, gall bladder, harderian and lacrimal gland, larynx, mammary gland, salivary gland, tongue, toe ureter, urethra<br><br>Category IV<br>These organs are not found in humans and toxic lesions (noncarcinogenic) in these organs are not re extrapolable to humans.<br>Clitoral/preputial gland, zymbal's gland, anal glands |

# Table 4: Severity of Effect Measures

| Ranking Systems | Severity of Effect | | |
|---|---|---|---|
| Examination of the Severity of Toxic Effects and Recommendation of a Systematic Approach to Rank Adverse Effects (USEPA 1986, prepared for ECAO, March) | *Organ*<br>Loss of which is fatal and are irreplaceable (I)<br>= 1.5<br>Loss of which may be fatal yet are replaceable or organs which is necessary for proper function of immunity (II)<br>= 1.0<br>Loss of which is not fatal but may result in functional or emotional handicap (III)<br>= 0.5<br>Not found in humans and toxic lesions found may not transfer to humans (IV)<br>= 0.25 | *Histopathological Severity*<br>No change<br>= 1.0<br>Effects evident only at EM level<br>= 2.0<br>Swelling, degeneration, fatty change, pigment<br>= 3.0<br>Atrophy, hypertrophy, cytomegaly, homorrhage<br>= 4.0<br>Necrosis, mineralization, emphysema, infarction<br>= 5.0<br>Fibrosis/regeneration, atypia hyperplasia/proliferation<br>= 6.0<br>Teratogenesis with maternal toxicity, fetotoxicity w/o maternal toxicity<br>= 7.0<br>Teratogenesis w/o maternal toxicity<br>= 8.0 | *Toxicity Endpoint*<br>Body wt. change, food and/or water cons. change, impairment of organs (IV)<br>= 1.0<br>Small hematological changes, impairment of organs (III), weight change in organs (II, III, IV)<br>= 2.0<br>mild impairment of organs (II), severe impairment of organs (III), minor organ weight change (I)<br>= 3.0<br>mild impairment of organs (I), major impairment of organs (II), major organ weight change (I)<br>= 4.0<br>Functional impairment of organs (I),<br>= 5.0<br>Major degree of funct'l impairment in organs (I)<br>= 6.0<br>Nervous System, respiratory, or cardiovascular depression, mortality, developmental toxicity w/o maternal toxicity<br>= 7.0 |

d. Factoring data quality/uncertainty into the index

There are differences among chemicals in the supporting health effects and exposure data. Health data for one type of effect (e.g., cancer) may be based on animal studies, while evidence of other types of effects may be derived from epidemiology (e.g. neurological effects of lead). Even specific numerical estimates of a single type of effect, cancer potency, have varying levels of evidence to support the estimate. For some chemicals without any specific toxicity data, we may have to use structure-activity relationships to estimate the relative rankings. There will also be differences in levels of uncertainty associated with exposure scenarios. For example, we may be able to model air and water emissions from certain facilities, but have less information on releases from TSDFs and POTWs.

The only system we reviewed that attempted to measure and incorporate any element of data uncertainty was the method for determining carcinogenicity RQ. This system employs an ordinal scoring for carcinogenic weight-of-evidence. This score is combined with a score based on $q_1^*$ using a matrix in which each cell is assigned a high, medium or low rank. This same approach could be used to weight ranks in the noncancer toxicity categories, as well as in exposure categories. Alternatively, numerical uncertainty scores could be used to weight chemical scores within a category.

e. Using severity indices to weight chemical scores within a category

Several systems develop human health effects scores that are comparable across different kinds of non-cancer risks. These systems employ effect severity indices to weight different effects by the relative risks they pose. For example, a report done for EPA/ECAO develops two scales that ordinarily rank noncarcinogenic toxic effects, one by lesion severity, another by type of effect. Both scales rank the effects relative to each other, but do not measure the magnitude of the overall risk. No attempt was made to rank these effects relative to cancer; nor did the report focus on reproductive or mutagenic effects. These scales would therefore be useful for ranking only noncarcinogenic human health risks.

f. Ranking individual chemicals or forming subindices

Once chemicals are scored relative to one another within each category, each chemical can be characterized by its profile of scores. At this point, a chemical's scores can be combined across categories to form a rank for that chemical in each area of interest (i.e. human health risks, environmental risks.) These ranks would be used to calculate the index. One advantage to this method is that such ranks indicate the relative importance of a chemical with a single number. Many systems, however, do not aggregate scores across categories (see the Region 7 and the OTS/ORNL scoring systems) because this requires making the difficult judgement about the relative importance of risks posed by different categories.

. Alternatively, scores can be aggregated within a category across chemicals to form a category subindex. For example, mammalian acute toxicity scores of all chemicals might be

added together (possibly weighted by exposure scores) to calculate the 'mammalian acute toxicity subindex.' This could be done for each category, creating an aggregate profile of all of the TRI chemicals. Movements within these subindices would provide measures of environmental improvement.

g. Methods of establishing the relative importance of risks among categories

If a single rank is to be calculated for each chemical from the various categorical scores, one of several calculation methods could be used. The simplest ways to combine numerical scores is to multiply or add them together. The flaw in this approach is that ordinal scores have no specific numerical meaning except within the categories, and even then they do not reflect the magnitude of the differences, but only the order of the ranks (see above.)

Another approach is to scale the scores then multiply or add them together so that the scores have a common denominator. For example, we could divide the exposure value at a facility by the maximum exposure value observed over all facilities. We can then add the scores in different categories because they have a similar scale.

A third approach is to create a matrix of categories and then rank each cell of the matrix separately. The cells may (but do not have to) reflect a mathematical function of the individual ranks of row and column that make up the cell. In this approach, individual chemicals would not be ranked; only the categories into which they fell would have ranks. This method is particularly appropriate for combining several qualitative (i.e. high, medium, low) scores. For example:

| Aquatic Risk Rank | | Persistence | | | |
|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 3 |
| Acute Aquatic Toxicity | Low | 0 | 0 | 0 | 0 |
| | Medium | 3 | 6 | 9 | 12 |
| | High | 6 | 9 | 12 | 15 |
| | Very High | 9 | 12 | 15 | 18 |

A fourth option is simply to select the worst score that a chemical has in any category and use that value as the chemical's rank. This would require that all of the scores be of the same type, i.e. qualitative or numerical. It also implies that scales of the scores can be equated. The methods for determining scores in each of the categories would have to meet these criteria.

Ranks in one category could also be conditional on a rank in a different category. For example, noncarcinogenic chronic toxicity might only be meaningful if exposure is above threshold RfD. Criteria for ranking a chemical might require that the noncarcinogenic toxicity score and exposure score meet separate criteria at the same time.

We can also apply special decision rules in conjunction with the overall scoring system. This may be useful in cases in which a particular score category is of overwhelming importance given certain conditions. For example, an extreme carcinogenicity score, regardless of other scores, might automatically classify a chemical as "high". A *de minimis* emissions score might eliminate the chemical from further consideration regardless of toxicity scores. Chemicals with very low toxicity in all categories might also be eliminated.

h. Weighting scores: an alternative to methods presented in I.g.

One option discussed in Section I.e. was to combine scores across categories to derive a single score for the chemical. A scoring algorithm to combine a chemical's scores across categories into a single rank requires the assignment of weights to each of the scoring elements. This is probably the most controversial and difficult step in the process because of the difficulty in evaluating the relative importance of different kinds of risk. In fact, some of systems we reviewed avoided this step altogether. However, in order to develop a single index that encompasses different kinds of risk (e.g. a human health index which incorporates both carcinogenic and noncarcinogenic risks), a weighting system which implies relative importance of effects will have to be used.

The primary issue in comparing two risks of different nature centers on attributing a common unit of value to the risks so that their relative magnitude can be compared. Of the EPA and non-EPA ranking systems reviewed under this assignment, only the Office of Toxic Substances Production-Based Targeting Methodology explicitly assigns relative values to different kinds of risks. Risks from oncogenicity, reproductive and neurotoxicity, chronic toxicity, and ecotoxicity were assigned relative weights of 3, 1, 2 and 2, respectively. Outside of the Agency, Louisiana's Environmental Action Plan gave equal weight to human cancer and non-cancer risks.

Other ranking systems implicitly weight different toxicity risks. For example, RQs indirectly address disparate risk comparisons by restricting the possible scores depending on the particular RQ being developed: cancer RQs can only range from 1-100, while aquatic toxicity RQs can range from 1-5000. The Hazard Ranking System employs a toxicity scale from 0 to 10,000 that enters into the calculation of site ranking without adjustment for the kind of toxic risk measured. The scale is based on various measures depending on the kind of toxicity being incorporated:

| Human Chronic Toxicity | Human Carcinogenicity | | | Acute Human Toxicity | | | | Assigned Value |
|---|---|---|---|---|---|---|---|---|
| Reference dose (RfD) (mg/kg-day) | Weight-of-Evidence and Slope Factor (SF) (mg/kg-day) | | | Oral $LD_{50}$ (mg/kg) | Dermal $LD_{50}$ (mg/kg) | Dust or mist $LC_{50}$ (mg/l) | Gas or Vapor $LC_{50}$ (ppm) | |
| | A | B | C | | | | | |
| < 0.0005 | 0.5 < | 5 < | 50 < | NA | NA | NA | NA | 10,000 |
| 0.0005 to 0.005 | 0.5 to 0.05 | 5 to 0.5 | 50 to 5 | < 5 | < 2 | < 0.2 | < 20 | 1,000 |
| 0.005 to 0.05 | < 0.05 | 0.5 to 0.05 | 5 to 0.5 | 5 to 50 | 2 to 20 | 0.2 to 2 | 20 to 200 | 100 |
| 0.05 to 0.5 | NA | < 0.05 | < 0.5 | 50 to 500 | 20 to 200 | 2 to 20 | 200 to 2,000 | 10 |
| 0.5 < | NA | NA | NA | 500 < | 200 < | 20 < | 2,000 < | 1 |

This system implies that risk from a class B carcinogen with a slope factor between 5 and 0.5 is ten times greater than the risk posed by a chronic toxic effect with an RfD between 0.005 and 0.05. The 307(a) Priority Pollutant Chemical Ranking System employs a similar method to develop toxicity scores.

There are also several approaches described in the economics literature that could be used to develop the relative severity ranking. First, economists use various techniques to determine the willingness to pay to avoid various health effects. Other studies examine direct risk/risk tradeoffs. One methodology involves asking respondents to choose between a number of hypothetical scenarios, two at a time. A point of indifference can be established between two scenarios through multiple iterations of questioning. This value determines a relative weight for the health effect being measured. Another method, the health status index, measures health effects in terms of changes in quality of life. While the scope of this project does not allow for original research, we could examine the available economics literature for results that would be applied in this context.

## II. Options for Ranking of Chemicals

Section I has described the elements of a scoring system. The components described in that section can be combined in numerous ways to produce an index. The following is a discussion of three possible options. **The options presented below should in no way be considered the universe of possible options.** Rather, they should be considered as points of departure for discussion of an appropriate algorithm for constructing the TRI index. The elements of each of the options were drawn from (or are modifications of) scoring systems discussed in our review memorandum entitled "Previous Work on Scoring Systems and Chemical Indices." However, none of the options presented below follows one system in its entirety; the specific combinations of components are original to this exercise. Option 1 ranks chemicals ordinally, based on selected measures of the toxicity and exposure potential of a chemical. These ranks are combined with population and emissions data to determine the final TRI indicator. Option 2 takes the same general approach but instead of ordinal ranks uses actual toxicity data values to develop unique rankings for each chemical. Option 2 also uses modelling to evaluate exposure potential. Option 3 describes an approach where categories of chemicals are defined based on relevant toxicity and exposure potential combinations. The categories (rather than the chemicals themselves) are assigned relative ranks. Chemicals are then assigned to the categories. Site-specific population and emissions data are then combined with the categorical ranks to calculate the indicator.

Step-by-step descriptions of each of these options are presented below. For each step, we identify previous EPA or other scoring systems that have used similar approaches. Summarizes of other EPA and non-EPA scoring systems are presented in the memorandum entitled "Previous Scoring and Ranking Systems" (hereafter referred to as the scoring system review memo). To illustrate the use of these options, we have created a sample data set of six hypothetical chemicals and three hypothetical facilities. The chemical-specific and site-specific data for these six chemicals are shown in Tables 5 and 6. For each of the options proposed, we provide an example of how the indicator would be constructed based on the sample data set.[2] The sample data set is kept simple intentionally, since our current focus is the conceptual structure of the indicator rather than the vagaries of our data set. Furthermore, we have generalized the discussion of evaluating potential; more detail on the mechanics of evaluating exposure potential is provided in the memorandum entitled "Mechanics of Evaluating Exposure for the TRI Index." Of course, the actual data set will be far more complicated, uncertain and incomplete than the sample data presented here. Once the Work Group has had the opportunity to review and discuss the conceptual approaches, we can explore the details of implementing potential options using an actual subset of the TRI data set.

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[2] While the examples provided show how a human-health based indicator would be developed, the same principles can be applied to the development of an ecological indicator.

## TABLE 5 - CHEMICAL-SPECIFIC DATA

| Chemical | Toxicity Data | | | | Physicochemical Data | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | Cancer | | Chronic Toxicity Other Than Cancer | | Volatility | | Partitioning | | | Persistence | |
| | WOE | q1* (kg-day/mg) | RfD (mg/kg-day) | Chronic Effect of Concern | Vapor Pressure (torr) | Henry's Law Constant (atm-m3/mol) | Koc (cm3/g) | BCF | Solubility (mg/l) | Photolysis (1/hr) | Hydrolysis (1/hr) |
| A | B2 | 10 | 0.1 | liver hypertrophy | 3.00E+03 | 2.00E-07 | 4.00E+01 | 10 | 4.00E+05 | 5.00E-03 | 6 80E-05 |
| B | B2 | 0.001 | 0.2 | nerve damage | 1.00E+02 | 2.00E-02 | 2.00E+02 | 50 | 8.00E+02 | 3 00E-08 | 4 00E-08 |
| C | B2 | 1 | 0.02 | spontaneous abortion | 4.00E-03 | 1.00E-05 | 1.10E+03 | 200 | 5.00E+00 | 4 00E-03 | 4 00E-02 |
| D | A | 0 03 | 0.05 | liver toxicity | 4.00E-04 | 1.00E-03 | 3.00E+03 | 1000 | 2.00E-01 | 1 00E-05 | 7 00E-03 |
| E (metal) | C | 5 | 0.005 | slowed neural response | 0 | 0 | na | 0 | 5.00E-01 | 0 | 0 |
| F (metal) | B2 | 45 (I) | 0.001 | decreased spermatogenesis | 0 | 0 | na | 0 | 5.00E+01 | 0 | 0 |

**TABLE 6 - SITE-SPECIFIC EXPOSURE DATA**

| Facility and Chemicals | Emissions | | Population Exposed | | Characteristics of Facility | |
|---|---|---|---|---|---|---|
| | Air (lbs/yr) | Water (lbs/yr) | Air (no. people) | Water (no. people) | Air | Water |
| **Facility 1** | | | | | | |
| A | 1000 | 6000 | 3000 | 500 | | Low |
| B | 2000 | 4000 | 3000 | 500 | High | Stream |
| C | 2000 | 1000 | 3000 | 500 | Dispersion | Flow |
| E | 4000 | 3000 | 3000 | 500 | | |
| **Facility 2** | | | | | | |
| C | 3000 | 1000 | 1000 | 6000 | | Medium |
| D | 4000 | 5000 | 1000 | 6000 | Low | Stream |
| F | 10000 | 2000 | 1000 | 6000 | Dispersion | Flow |
| **Facility 3** | | | | | | |
| A | 2000 | 4000 | 2000 | 2000 | | High |
| C | 4000 | 2000 | 2000 | 2000 | Medium | Stream |
| D | 6000 | 10000 | 2000 | 2000 | Dispersion | Flow |
| E | 1000 | 6000 | 2000 | 2000 | | |

Option 1.

**Step 1. Using an ordinal scale, rank chemicals within each toxicity evaluation criterion.** Ordinal ranking is a common approach in a number of ranking systems. Often, ranks are assigned on an ordinal scale (from 0-10, for example) rather than assigning unique values to each chemical. The ranking of the chemicals is based on quantitative dose-response information if possible. Several systems we reviewed used ordinal scales for ranking toxicity, including the TRI Risk Screening Guide, OTS pollution prevention screening, the OTS/ORNL chemical ranking scheme, and the Louisiana Environmental Action Plan.

**Step 2a. Within each of these toxicity categories, assign severity rank (e.g., cellular change versus organ damage) for noncarcinogens.** Chemicals that have similar reference doses may pose dissimilar health risks. Severity ranking attempts to weight chemicals based on the relative gravity of the noncancer health effects risks posed. Severity ranking has been used in several previous ranking/scoring efforts, such as the OTS pollution prevention screening, the Integrated Environmental Management Program, and the Louisiana Environmental Action Plan. A scheme for severity ranking was presented in the ECAO report entitled "Examination of the Severity of Toxic Effects and Recommendations of a Systematic Approach to Rank Adverse Effects," which is presented in detail in the scoring systems review memo.

**Step 2b. Assign ranks based on weight-of-evidence (e.g., substantial evidence versus suggestive evidence) ranks for carcinogens.** This step is an attempt to recognize the uncertainty in the classification of a chemical as a human carcinogen. This step uses the CAG weight- of-evidence (WOE) classification scheme (where A = known human carcinogen; B = probable human carcinogen; and C = possible human carcinogen) to weight carcinogens. Ranking based on weight-of-evidence classification has been used in the OTS pollution prevention screening and in the Integrated Environmental Management Program, and has played a role in other schemes that use "best professional judgment" to assign ranks to chemicals (such as the Unfinished Business report).

**Step 3. Determine relative weights for each toxicity category relative to other categories (e.g., hepatic effects versus cancer).** This is likely to be among the most controversial steps in the process. Many scoring systems have avoided combining dissimilar risks and have instead developed separate scores for different types of risks. For example, the Region VII TRI strategy is to derive separate indices for chemicals based on acute effects, chronic noncancer, cancer and aquatic toxicity. However, a few weighting schemes (notably, two regulatory efforts) have compared different types of toxicity. The Hazard Ranking System (used to place sites on the NPL) implicitly assigns relative weights to cancer and non-cancer effects by using the same scale to score chemicals on these attributes (see the scoring systems review memo for further detail). Also, OAQPS has proposed a scheme for establishing off-setting emissions credits in the program governing early emissions reductions of hazardous air pollutants. The scheme explicitly allows emissions trading among

carcinogens and other chemicals, where emissions from carcinogens are (numerically) weighted more heavily than noncarcinogens.

**Step 4. The categorical toxicity rank for each chemical is the product of the raw toxicity rank, the severity/WOE rank and the categorical rank. The overall toxicity rank for a chemical is the average of its ranks in the four toxicity categories.** Another possible approach would be to take the root mean square of the four toxicity category ranks (an approach used in the Hazard Ranking System).

**Step 5. For the exposure evaluation criteria, use photolysis rate, solubility, and bioconcentration factor to rank chemicals for the inhalation, drinking water, and fish ingestion exposure pathways, respectively.** A number of systems use relevant physicochemical values to evaluate exposure potential in various media. The Risk Screening Guide used selected physicochemical parameters to qualitatively evaluate mobility of chemicals in each media. The Hazard Ranking System also uses selected parameters to score exposure potential, although a greater number of parameters are included in the HRS exposure evaluation because some site-specific data are generally available for HRS evaluations.

**Step 6. Multiply the media-specific exposure rank and toxicity rank by population exposed and emissions for that pathway for each facility.** This step combines the toxicity considerations with the factors that determine exposure potential (i.e., the chemical's exposure rank and emissions, and population size). Size of exposed population is used as a ranking criteria in many of scoring systems we reviewed, including: the PPD TRI pollution prevention targeting; OPA ranking of discharges to POTWs and surface waters; OTS TSCA prescreening of TRI chemicals; the Hazard Ranking System; the Integrated Environmental Management Program; the Louisiana Environmental Action Plan; and the California Air Toxics Hotspots Program.

The use of population size as a prominent weighting factor may be unacceptable to those who feel that such an emphasis undervalues risks to rural populations. Furthermore, various regulatory efforts in the Agency focus risks to the Most Exposed Individual (MEI); a TRI indicator method which does not consider MEI risks would conflict with this philosophy. There are also difficulties associated with characterizing the size of exposed populations for certain exposure pathways (such as solid waste disposal). These difficulties will result in unequal levels of uncertainty in the exposure potential evaluation across exposure pathways.

On the other hand, overall population risk has been used elsewhere (notably, in the Unfinished Business report) to characterize general environmental progress; avoidance of population risk, not MEI risk, is also used in cost-benefit analyses to describe potential benefits of implementing environmental regulations.

**Step 7. The final index is the sum of the weighted volumes for all TRI chemicals for all pathways across all facilities.**

A step-by-step example demonstrating Option 1 for the sample data set is found in **Figure 1.**

**Advantages** - This option allows fine-scale tracking of subtle differences among chemicals. Importantly, by calculating media-chemical-facility subindices, we can easily identify underlying reasons for changes in the overall index by tracking individual media, industries, or chemicals. However, the final calculation yields a single index rather than a series of subindices across categories that may be hard for the public to interpret.

**Disadvantages** - Determining appropriate and sensible weighting factors for the different elements is difficult. Retaining a proportional scoring system based largely on ordinal ranks and performing mathematical functions on them may give the false impression that the absolute magnitude of the ranks have numerical meaning.

Figure 1. Example Calculation for Option 1 Ranking System

Step 1. Using an ordinal scale, rank chemicals within each selected toxicity evaluation criteria.

For this and subsequent steps, ranks are ordered low to high.

| Chemical | Cancer | Chronic Toxicity Other Than Cancer | | |
|---|---|---|---|---|
| | | Liver | Neurologic | Reproductive |
| A | 5 | 1 | | |
| B | 1 | | 1 | |
| C | 3 | | | 1 |
| D | 2 | 2 | | |
| E (metal) | 4 | | 2 | |
| F (metal) | 6 | | | 2 |

Step 2. Within each of these categories, assign severity and weight of evidence rank to each chemical.

2.a. For this step, we use weights from 1 to 3 to rank the relative severity of chronic effects.

| Chemical | Chronic Toxicity Other Than Cancer | | |
|---|---|---|---|
| | Liver | Neurologic | Reproductive |
| A | 1 | | |
| B | | 3 | |
| C | | | 2 |
| D | 3 | | |
| E (metal) | | 1 | |
| F (metal) | | | 1 |

2 b We use weights from 1 to 3 for assigning carcinogens by their weight of evidence classification

| Chemical | Cancer (WOE) |
|---|---|
| A | 2 |
| B | 2 |
| C | 2 |
| D | 3 |
| E (metal) | 1 |
| F (metal) | 2 |

**Step 3. Determine weights for each toxicity category.**

**For the purposes of this example, the relative weights are:**

| | |
|---|---|
| **Cancer** | **10** |
| **Reproductive Effects** | **7** |
| **Neurological Effects** | **5** |
| **Other Chronic Effects** | **2** |

**Step 4. Derive categorical toxicity rank by multiplying toxicity rank, effect-specific severity rank, weight of evidence rank and cross-category severity rank. To get overall rank, average the chemical's rank in each category.**

| Chemical | Cancer (a) | Chronic Toxicity Other Than Cancer (b) | | | OVERALL AVERAGE (a+b)/2 |
|---|---|---|---|---|---|
| | | Liver | Neurologic | Reproductive | |
| A | 5 x 2 x 10 = 100 | 1 x 1 x 2 = 2 | | | 51 |
| B | 1 x 2 x 10 = 20 | | 1 x 3 x 5 = 15 | | 17.5 |
| C | 3 x 2 x 10 = 60 | | | 1 x 2 x 7 = 14 | 37 |
| D | 2 x 3 x 10 = 60 | 2 x 3 x 2 = 12 | | | 36 |
| E (metal) | 4 x 1 x 10 = 40 | | 2 x 1 x 5 = 10 | | 25 |
| F (metal) | 6 x 2 x 10 = 120 | | | 2 x 1 x 7 = 14 | 67 |

Step 5 Derive rank for each exposure pathway based on salient physicochemical parameter

| Chemical | Air | Drinking Water | Fish Ingestion |
|---|---|---|---|
| | Based on Photolysis | Based on Solubility | Based on BCF |
| A | 1 | 6 | 3 |
| B | 4 | 5 | 4 |
| C | 2 | 3 | 5 |
| D | 3 | 1 | 6 |
| E (metal) | 5 | 2 | 1 |
| F (metal) | 5 | 4 | 1 |

Step 6 Combine exposure and toxicity ranks with population and emissions data to obtain media-specific indices.

FOR AIR:

| Facility | Chemical | Emissions (lbs/yr) (a) | Pop Exposed (no. people) (b) | Toxicity Rank (c) | Exposure Rank (d) | AIR INDEX e = a x b x c x d |
|---|---|---|---|---|---|---|
| Facility 1 | A | 1000 | 3000 | 51 | 1 | 1 5E+08 |
| Facility 3 | A | 2000 | 2000 | 51 | 1 | 2.0E+08 |
| Facility 1 | B | 2000 | 3000 | 17.5 | 4 | 4 2E+08 |
| Facility 1 | C | 2000 | 3000 | 37 | 2 | 4 4E+08 |
| Facility 2 | C | 3000 | 1000 | 37 | 2 | 2.2E+08 |
| Facility 3 | C | 4000 | 2000 | 37 | 2 | 5 9E+08 |
| Facility 2 | D | 4000 | 1000 | 36 | 3 | 4 3E+08 |
| Facility 3 | D | 6000 | 2000 | 36 | 3 | 1.3E+09 |
| Facility 1 | E | 4000 | 3000 | 25 | 5 | 1.5E+09 |
| Facility 3 | E | 1000 | 2000 | 25 | 5 | 2.5E+08 |
| Facility 2 | F | 10000 | 1000 | 67 | 5 | 3 4E+09 |
| TOTAL: | | | | | | |

**FOR WATER:**

**We obtain an average rank for water exposures using the following formula:**

**Total exposure to water sources is expressed as : 2L drinking water + [0.14 kg fish *BCF (L/kg)]**

**Average rank for water = (Rank for drinking water x (2 L/total exp.)) + (Rank for fish x (0.14 x BCF)/total exp.)**

| Facility | Chemical | Emissions (lbs/yr) (a) | Pop Exposed (no. people) (b) | Toxicity Rank (c) | Drinking Water Exposure Rank (d) | Fish Ingestion Exposure Rank (e) | BCF Value (f) | Average Water Rank (g)=(d)x2L/tot exp +(e)x0.14(f)/tot exp | WATER INDEX h = a x b x c x g |
|---|---|---|---|---|---|---|---|---|---|
| Facility 1 | A | 6000 | 500 | 51 | 6 | 3 | 10 | 5 | 7.3E+08 |
| Facility 3 | A | 4000 | 2000 | 51 | 6 | 3 | 10 | 5 | 1.9E+09 |
| Facility 1 | B | 4000 | 500 | 17.5 | 5 | 4 | 50 | 4 | 1 5E+08 |
| Facility 1 | C | 1000 | 500 | 37 | 3 | 5 | 200 | 5 | 9 0E+07 |
| Facility 2 | C | 1000 | 6000 | 37 | 3 | 5 | 200 | 5 | 1 1E+09 |
| Facility 3 | C | 2000 | 2000 | 37 | 3 | 5 | 200 | 5 | 7 2E+08 |
| Facility 2 | D | 5000 | 6000 | 36 | 1 | 6 | 1000 | 6 | 6 4E+09 |
| Facility 3 | D | 10000 | 2000 | 36 | 1 | 6 | 1000 | 6 | 4 3E+09 |
| Facility 1 | E | 3000 | 500 | 25 | 2 | 1 | 0 | 2 | 7.5E+07 |
| Facility 3 | E | 6000 | 2000 | 25 | 2 | 1 | 0 | 2 | 6 0E+08 |
| Facility 2 | F | 2000 | 6000 | 67 | 4 | 1 | 0 | 4 | 3 2E+09 |
| TOTAL: | | | | | | | | | 1 9E+10 |

Step 7 Sum media-specific indices for overall TRI index

| Facility | Chemical | AIR INDEX (a) | WATER INDEX (b) | TOTAL TRI INDEX c = (a+b) |
|---|---|---|---|---|
| Facility 1 | A | 1.5E+08 | 7.3E+08 | 8.8E+08 |
| Facility 3 | A | 2.0E+08 | 1.9E+09 | 2.1E+09 |
| Facility 1 | B | 4.2E+08 | 1.5E+08 | 5.7E+08 |
| Facility 1 | C | 4.4E+08 | 9.0E+07 | 5.3E+08 |
| Facility 2 | C | 2.2E+08 | 1.1E+09 | 1.3E+09 |
| Facility 3 | C | 5.9E+08 | 7.2E+08 | 1.3E+09 |
| Facility 2 | D | 4.3E+08 | 6.4E+09 | 6.8E+09 |
| Facility 3 | D | 1.3E+09 | 4.3E+09 | 5.6E+09 |
| Facility 1 | E | 1.5E+09 | 7.5E+07 | 1.6E+09 |
| Facility 3 | E | 2.5E+08 | 6.0E+08 | 8.5E+08 |
| Facility 2 | F | 3.4E+09 | 3.2E+09 | 6.6E+09 |
| TOTAL | | 8.9E+09 | 1.9E+10 | 2.8E+10 |

**Option 2.**

**Step 1. Rank chemicals using actual proportional measures for the categories of concern.** For carcinogens, use $q_1^*$ values. The $q_1^*$ expresses risk to an individual per milligram (mg) of chemical per kilogram of body weight per day (mg/kg-day). For noncarcinogens, use the inverse of the RfD. The RfD is the dose (expressed as mg of chemical per kg body weight per day) below which no adverse effects are expected to occur. Using proportional measures for toxicity ranking is a common approach in other ranking systems. For example, RQs were used by OPA in ranking discharges to POTWs and to surface water bodies; OTS TSCA prescreening of TRI chemicals used RQ as a cutoff for high concern chemicals. RfDs and $Q^*$ are proposed as the basis for toxicity ranking in Region VII's TRI strategy. Outside the Agency, the California Air Toxic Hotspots program uses actual dose-response data (in conjunction with exposure modelling - discussed below) in their identification and ranking of air toxics problems in the state.

**Step 1a. Since toxicity values in different categories have dissimilar units (e.g., cancer potency estimate versus an RfD), normalize the values by expressing the chemical's toxicity value in a given category as a fraction of the maximum value possible in that category.** The resulting fraction is the chemical's rank in that category. Expressing the ranks in this manner will also allow us to combine the ranks with exposure potential ranks that have been normalized in a similar manner (see below). This normalizing approach was used in OAQPS' Source Category Ranking System, which ranks potential air toxics problems across industries.

Once the toxicity ranks within categories are determined, the next three steps are the same as those described in Option 1.

**Step 2a and 2b. Within each toxicity category, assign severity and weight-of-evidence (WOE) ranks to each chemical.**

**Step 3. Determine relative weights for each toxicity category relative to other categories.**

**Step 4. Determine the categorical toxicity rank for each chemical. The categorical rank is the product of the raw toxicity rank, the severity rank, the WOE rank and the categorical rank. The overall toxicity rank is the average of its ranks in the four toxicity categories.**

**Step 5. For the exposure evaluation, model the fate and transport of the chemicals.** To do so, use the emissions data, site-specific environmental characteristics (or default values where these are not available), and physicochemical properties to obtain ambient media concentrations at specified distances. These data can be weighted by the number of persons at each distance (that is, the number of persons exposed to each estimated concentration) to obtain population-weighted average exposures for each site where chemical is emitted.

As mentioned earlier, specific methods for applying exposure modelling to the TRI database are discussed in a separate memo and will not be expanded on here. However, it should be noted that generic exposure modelling to rank exposure potential is used by a number of other scoring/ranking systems. For example, Appendix B of the Risk Screening Guide presents results of generic air modelling to assist readers in the evaluation of air releases. OTS' TSCA prescreening of TRI chemicals used generic air and water exposure modelling to place chemicals in categories of low, medium and high concern. Furthermore, generic air modelling was used by OAQPS to identify high risk chemicals as part of defining offsets credits for early emissions reductions of hazardous air pollutants. Other scoring methods using generic modelling approaches include the California Air Toxics Hotspots program and OAQPS' Source Category Ranking System.

**Step 6. For each chemical-facility combination, express the exposure estimate as a fraction of the maximum exposure observed to obtain an exposure index.** Normalizing the exposure values allows us to combine the exposure ranks with the toxicity rankings in later steps. Otherwise, we would be combining ranks with dissimilar scales. The exposure index is then combined with the toxicity rank to derive the medium-specific index. The final index is the sum of the media-specific indices.

(A modification to this approach would be to use the RfDs and $q_1^*$s in concert with the exposure models to estimate cancer cases and/or number of individuals above the RfD. The "cases" could then be scaled by the maximum number of "cases" observed at each facility to obtain a unique subindex for each chemical-facility combination by exposure pathway. The index for the chemical would be the sum of the subindices across all facilities. The overall index would be the sum of the chemical indices.)

An example demonstrating Option 2 for the sample data set is found in **Figure 2.**

**Advantages** - The use of location-dependent exposure indices allows the index to reflect changes in where chemicals are released, as well as changes in volume. Normalizing toxicity ranks allows the use of structure-activity relationships to fill in data gaps; if a particular toxicity value is not known, the chemical can still be assigned a rank relative to the highest value in the category.

**Disadvantages** - The lack of toxicity data for many of the TRI chemicals would hinder this approach. This approach presents some programming challenges for performing multiple chemical, multiple site analyses. This option has the same difficulties as Option 1 in assigning appropriate sensible weighting factors to different elements. Furthermore, the option relies on normalizing the ranks based on a "reference chemical" which has the maximum value in the ranking category. A danger in this approach is the possibility that the underlying data (toxicity or physicochemical information) may change over time. Since all other chemical ranks are keyed to the values for this chemical, a change in the reference chemical would change the entire index. Therefore, rather than selecting the chemical with the maximum value, we may want to select as the reference chemical a well-known, well

characterized chemical for which underlying data is unlikely to change. Using this approach, the reference chemical rank would still be 1, while chemicals with values greater than the reference chemical would be assigned ranks proportionally greater than 1.

Figure 2. Example Calculation for Option 2 Ranking System

**Step 1. Using inverse of RfD value and actual q* values, rank chemicals within each selected toxicity evaluation criteria.**

For this and subsequent steps, ranks are ordered low to high.

| Chemical | Cancer (q*) | Chronic Toxicity Other Than Cancer (1/RFD) | | |
|---|---|---|---|---|
| | | Liver | Neurologic | Reproductive |
| A | 10 | 10 | | |
| B | 0.001 | | 5 | |
| C | 1 | | | 50 |
| D | 0.03 | 20 | | |
| E (metal) | 5 | | 200 | |
| F (metal) | 45 | | | 1000 |

**Step 1a. Since the raw toxicity ranks are on different scales, express the rank in each category as a fraction of the maximum rank observed in that category. The maximum rank is 1.**

| Chemical | Cancer | Chronic Toxicity Other Than Cancer | | |
|---|---|---|---|---|
| | | Liver | Neurologic | Reproductive |
| A | 2.2E-01 | 0.5 | | |
| B | 2.2E-05 | | 0.025 | |
| C | 2.2E-02 | | | 0.05 |
| D | 6.7E-04 | 1 | | |
| E (metal) | 1.1E-01 | | 1 | |
| F (metal) | 1.0E+00 | | | 1 |

Step 2 Within each of these categories, assign severity and weight of evidence rank to each chemical.

2.a. As in Option 1, we use weights from 1 to 3 to rank the relative severity of chronic effects.

| Chemical | Chronic Toxicity Other Than Cancer | | |
|---|---|---|---|
| | Liver | Neurologic | Reproductive |
| A | 1 | | |
| B | | 3 | |
| C | | | 2 |
| D | 3 | | |
| E (metal) | | 1 | |
| F (metal) | | | 1 |

2.b. We use weights from 1 to 3 for assigning carcinogens by their weight of evidence classification.

| Chemical | Cancer (WOE) |
|---|---|
| A | 2 |
| B | 2 |
| C | 2 |
| D | 3 |
| E (metal) | 1 |
| F (metal) | 2 |

Step 3. Determine severity weights for each toxicity category.

This step is also the same as Option 1. For the purposes of this example, the relative weights are:

| | |
|---|---|
| Cancer | 10 |
| Reproductive Effects | 7 |
| Neurological Effects | 5 |
| Other Chronic Effects | 2 |

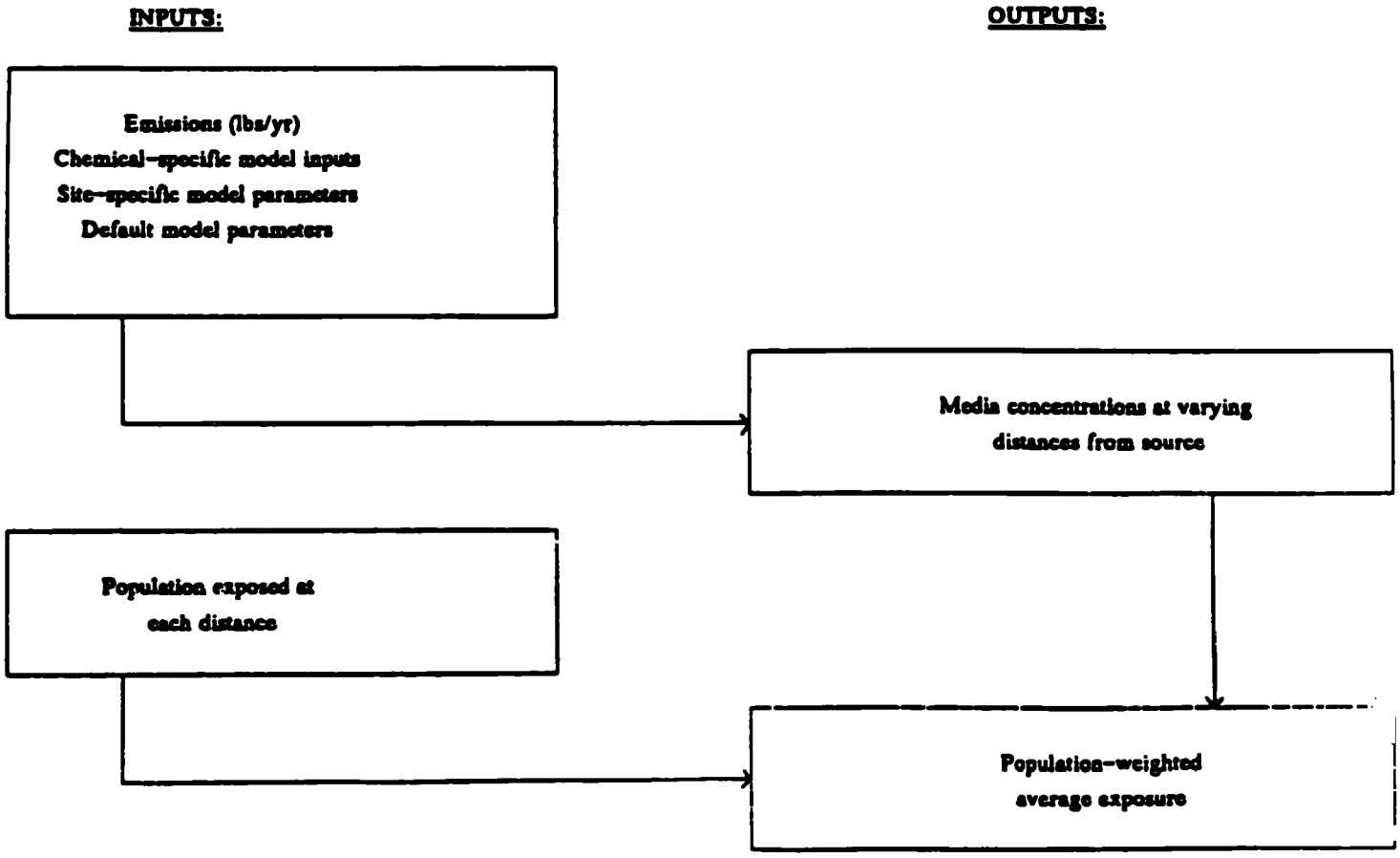
Step 4 Derive categorical toxicity rank by multiplying toxicity rank, severity rank and category rank. To get overall rank, average the chemical's rank in each category.

| Chemical | Cancer (a) | Chronic Toxicity Other Than Cancer (b) | | | OVERALL AVERAGE (a+b)/2 |
|---|---|---|---|---|---|
| | | Liver | Neurologic | Reproductive | |
| A | 2e-1 x 2 x 10 = 4 | 0.5 x 1 x 2 = 1 | | | 2.7 |
| B | 2e-5 x 2 x 10 = 4e-4 | | 0.025 x 3 x 5 = 4e-1 | | 0.2 |
| C | 2e-2 x 2 x 10 = 4e-1 | | | 0.05 x 2 x 7 = 7e-1 | 0.6 |
| D | 7e-4 x 3 x 10 = 2e-2 | 1 x 3 x 2 = 6 | | | 3.0 |
| E (metal) | 1e-1 x 1 x 10 = 1 | | 1 x 1 x 5 = 5 | | 3 1 |
| F (metal) | 1 x 2 x 10 = 20 | | | 1 x 1 x 7 = 7 | 13.5 |

Step 5. Derive rank for each exposure pathway using modelling approach.

For this step, we use computer programs to estimate population-weighted average in each medium, for each chemical at each facility.

The steps are as follows:



For the purposes of this example, we assume that these models yield the following results.

**FOR AIR:**

| Facility | Chemical | Emissions (lbs/yr) | Pop. Exposed (no. people) | Population-Weighted Average Exposure (calculated with model) |
|---|---|---|---|---|
| Facility 1 | A | 1000 | 3000 | 5.0E-04 |
| Facility 3 | A | 2000 | 2000 | 3.3E-03 |
| Facility 1 | B | 2000 | 3000 | 9.0E-03 |
| Facility 1 | C | 2000 | 3000 | 2.0E-03 |
| Facility 2 | C | 3000 | 1000 | 3.3E-03 |
| Facility 3 | C | 4000 | 2000 | 8.0E-03 |
| Facility 2 | D | 4000 | 1000 | 3.3E-02 |
| Facility 3 | D | 6000 | 2000 | 2.0E-02 |
| Facility 1 | E | 4000 | 3000 | 2.0E-02 |
| Facility 3 | E | 1000 | 2000 | 1.7E-02 |
| Facility 2 | F | 10000 | 1000 | 1.7E-01 |

**FOR WATER:**

| Facility | Chemical | Emissions (lbs/yr) | Pop Exposed (no. people) | Population-Weighted Average Exposure (calculated with model) |
|---|---|---|---|---|
| Facility 1 | A | 6000 | 500 | 3.5E-02 |
| Facility 3 | A | 4000 | 2000 | 9.4E-03 |
| Facility 1 | B | 4000 | 500 | 1.2E-02 |
| Facility 1 | C | 1000 | 500 | 2.9E-04 |
| Facility 2 | C | 1000 | 6000 | 7.1E-04 |
| Facility 3 | C | 2000 | 2000 | 4.7E-04 |
| Facility 2 | D | 5000 | 6000 | 2.8E-02 |
| Facility 3 | D | 10000 | 2000 | 4.7E-04 |
| Facility 1 | E | 3000 | 500 | 1.8E-04 |
| Facility 3 | E | 6000 | 2000 | 7.1E-03 |
| Facility 2 | F | 2000 | 6000 | 7.1E-02 |

Step 5a. Take the exposures as a fraction of the maximum in order to get exposure indices for the chemicals.

FOR AIR:

| Facility | Chemical | Exposure Index |
|---|---|---|
| Facility 1 | A | 3.0E-03 |
| Facility 3 | A | 2.0E-02 |
| Facility 1 | B | 5.4E-02 |
| Facility 1 | C | 1.2E-02 |
| Facility 2 | C | 2.0E-02 |
| Facility 3 | C | 4.8E-02 |
| Facility 2 | D | 2.0E-01 |
| Facility 3 | D | 1.2E-01 |
| Facility 1 | E | 1.2E-01 |
| Facility 3 | E | 1.0E-01 |
| Facility 2 | F | 1.0E+00 |

FOR WATER:

| Facility | Chemical | Exposure Index |
|---|---|---|
| Facility 1 | A | 5.0E-01 |
| Facility 3 | A | 1.3E-01 |
| Facility 1 | B | 1.7E-01 |
| Facility 1 | C | 4.2E-03 |
| Facility 2 | C | 1.0E-02 |
| Facility 3 | C | 6.7E-03 |
| Facility 2 | D | 4.0E-01 |
| Facility 3 | D | 6.7E-03 |
| Facility 1 | E | 2.5E-03 |
| Facility 3 | E | 1.0E-01 |
| Facility 2 | F | 1.0E+00 |

Step 6. To derive media-specific indices, multiply toxicity ranks and exposure indices.
To derive final index, add media-specific indices.

| Facility | Chemical | Air Exposure Index (from Step 5a) (a) | Toxicity Rank (from Step 4) (b) | AIR INDEX c=(axb) |
|---|---|---|---|---|
| Facility 1 | A | 3 0E-03 | 2.7 | 8 10E-03 |
| Facility 3 | A | 2.0E-02 | 2.7 | 2 72E+00 |
| Facility 1 | B | 5.4E-02 | 0.2 | 2.54E-01 |
| Facility 1 | C | 1.2E-02 | 0.6 | 6.12E-01 |
| Facility 2 | C | 2.0E-02 | 0.6 | 6 20E-01 |
| Facility 3 | C | 4.8E-02 | 0.6 | 6 48E-01 |
| Facility 2 | D | 2.0E-01 | 3 | 3 20E+00 |
| Facility 3 | D | 1.2E-01 | 3 | 3.12E+00 |
| Facility 1 | E | 1.2E-01 | 3.1 | 3.22E+00 |
| Facility 3 | E | 1.0E-01 | 3.1 | 3.20E+00 |
| Facility 2 | F | 1.0E+00 | 13.5 | 1.45E+01 |
| TOTAL: | | | | 32.1 |

| Facility | Chemical | Water Exposure Index (from Step 5b) (a) | Toxicity Rank (from Step 4) (b) | WATER INDEX c=(axb) |
|---|---|---|---|---|
| Facility 1 | A | 5.0E-01 | 2.7 | 1.35E+00 |
| Facility 3 | A | 1.3E-01 | 2.7 | 2.83E+00 |
| Facility 1 | B | 1.7E-01 | 0.2 | 3 67E-01 |
| Facility 1 | C | 4.2E-03 | 0.6 | 6 04E-01 |
| Facility 2 | C | 1.0E-02 | 0.6 | 6.10E-01 |
| Facility 3 | C | 6.7E-03 | 0.6 | 6.07E-01 |
| Facility 2 | D | 4.0E-01 | 3 | 3 40E+00 |
| Facility 3 | D | 6.7E-03 | 3 | 3.01E+00 |
| Facility 1 | E | 2.5E-03 | 3.1 | 3.10E+00 |
| Facility 3 | E | 1.0E-01 | 3.1 | 3.20E+00 |
| Facility 2 | F | 1.0E+00 | 13.5 | 1 45E+01 |
| TOTAL: | | | | 33 6 |

| Facility | Chemical | AIR INDEX (a) | WATER RANK (b) | OVERALL INDEX c=(a+b) |
|---|---|---|---|---|
| Facility 1 | A | 8 10E-03 | 1 35E+00 | 1.4 |
| Facility 3 | A | 2.72E+00 | 2 83E+00 | 5.6 |
| Facility 1 | B | 2.54E-01 | 3.67E-01 | 0.6 |
| Facility 1 | C | 6.12E-01 | 6.04E-01 | 1.2 |
| Facility 2 | C | 6.20E-01 | 6.10E-01 | 1.2 |
| Facility 3 | C | 6.48E-01 | 6.07E-01 | 1.3 |
| Facility 2 | D | 3.20E+00 | 3.40E+00 | 6.6 |
| Facility 3 | D | 3.12E+00 | 3.01E+00 | 6.1 |
| Facility 1 | E | 3.22E+00 | 3.10E+00 | 6.3 |
| Facility 3 | E | 3.20E+00 | 3.20E+00 | 6.4 |
| Facility 2 | F | 1.45E+01 | 1.45E+01 | 29.0 |
| TOTAL: | | 32.1 | 33.6 | 65.7 |

Option 3.

**Step 1. From among the various toxicity categories, choose the category which yields the lowest dose.** This is the limiting dose. This decision rule was used in the ranking of chemicals for inclusion as priority pollutants under the Clean Water Act.

**Step 2. Establish criteria for placing chemicals in categories of low, medium and high toxicity based on the limiting dose, and classify chemicals based on these criteria.** A number of scoring systems have provided criteria that could be used to place chemicals in categories of low, medium and high concern. The human and environmental toxicity categories into which chemicals were divided and the criteria used to place chemicals in these categories for each scoring system were summarized in Tables 1 and 2 of this memo.

**Step 3. To assess exposure potential, use photolysis rate, solubility, and bioconcentration factor for the inhalation, drinking water, and fish ingestion exposure pathways, respectively to place chemicals in categories of low, medium and high for exposure potential. Classify chemicals based on these criteria.** As with the toxicity ranking, a number of scoring systems have provided criteria that could be used to place chemicals in categories of low, medium and high exposure potential. The exposure potential categories into which chemicals were divided and the criteria used to place chemicals in these categories for each scoring system were summarized in Table 3 of this memo.

**Step 4. Construct human hazard and exposure potential matrices for each medium of concern; assign chemicals to each cell according to their toxicity and medium-specific classifications.** An example of such a matrix is given in ORD's "Simplified Approach for Screening and Categorizing Toxic Chemicals." A toxicity/exposure matrix was also used in the University of Michigan's application of the Hazard Ranking System to the prioritization of organic compounds at hazardous waste sites.

**Step 5. Assign weights to the low, medium and high categories for exposure potential and toxicity.** In our example, the rank for each cell in the matrix is the product of the toxicity weight and the exposure weight for the row and column that define the cell. The ORD simplified approach to classifying toxic chemicals provides an example of values assigned to matrix cells. OTS's TSCA prescreening of TRI chemicals also presents an exposure/toxicity matrix, but assigns ranks of low, medium or high to each cell, rather than numerical weights.

**Step 6. Individual chemical-facility indices are derived for each medium by multiplying the rank for the cell in which the chemical falls, the population exposed via that medium, and the emissions to that medium.**

**Step 7. The overall index is the sum of the media-specific indices across all chemicals and across all facilities.**

An example demonstrating Option 3 for the sample data set is found in **Figure 3.**

**Advantages** - This method avoids combining toxicity categories. It provides a simple but informative rank for each chemical based on a two-way classification scheme. The final index weightings are explicit and understandable.

**Disadvantages** - This approach assumes that all of the toxicity categories are of equal importance. In this approach, chemicals do not get specific exposure-toxicity ranks; only the categories to which they belong are ranked. The use of three broad categories within the scoring elements does not allow fine-scale differentiation among values for chemicals within a scoring element. This particular flaw would prevent us from distinguishing changes in chemicals with very high toxicities from changes in "border" chemicals with marginally high toxicities. Options to address this problem include (a) eliminating "border" chemicals from the index calculation; and (b) performing more explicit analysis on the "border" chemicals to evaluate how different the index would be if they switched into different categories.

Figure 3 Example Calculation for Option 3 Ranking System

Step 1. From among the toxicity criteria of interest, choose the lowest dose for each chemical among all the categories. This is the limiting dose.

| Chemical | Cancer | Chronic Toxicity Other Than Cancer | | | LIMITING DOSE |
|---|---|---|---|---|---|
| | | Liver | Neurologic | Reproductive | |
| | Risk-specific Dose at 1E-4 Risk Level (mg/kg-day) (1E-4/q*) | RfD (mg/kg-day) | RfD (mg/kg-day) | RfD (mg/kg-day) | (mg/kg-day) |
| A | 1E-05 | 1E-01 | | | 1E-05 |
| B | 1E-01 | | 2E-01 | | 1E-01 |
| C | 1E-04 | | | 2E-02 | 1E-04 |
| D | 3E-03 | 5E-02 | | | 3E-03 |
| E | 2E-05 | | 5E-03 | | 2E-05 |
| F | 2E-06 | | | 1E-03 | 2E-06 |

Step 2. Place chemicals into high, medium and low categories.

For this step, we need to develop criteria for what constitutes a high, medium or low toxicity. For the purposes of this example, we assign the following values to these categories:

| Category | Range |
|---|---|
| High | Dose < 1E-4 |
| Medium | 1E-4 < Dose < 1E-2 |
| Low | 1E-2 < Dose |

Using these criteria, we classify the chemicals:

| Chemical | LIMITING DOSE (mg/kg-day) | TOXICITY CATEGORY |
|---|---|---|
| A | 1E-05 | High |
| B | 1E-01 | Low |
| C | 1E-04 | Medium |
| D | 3E-03 | Medium |
| E | 2E-05 | High |
| F | 2E-06 | High |

**Step 3. Based on salient physicochemical properties, assign chemicals to high, medium and low exposure potential categories.**

For this step, we must establish media-specific criteria for assigning chemicals to high, medium and low categories.

For the purposes of this example, we make the following assignments:

| Exposure Medium | Criterion | | |
|---|---|---|---|
| | Low | Medium | High |
| Air | photolysis < 1E-7 | 1E-6 < photolysis ≤ 1E-4 | 1E-4 < photolysis |
| Drinking Water | solubility < 10 | 10 < solubility < 500 | 500 < solubility |
| Fish | BCF < 50 | 50<BCF < 500 | 500 < BCF |

Using these criteria, we classify the chemicals:

| Chemical | Air | Drinking Water | Fish |
|---|---|---|---|
| A | High | High | Low |
| B | Low | High | Medium |
| C | High | Low | Medium |
| D | Medium | Low | High |
| E | Low | Low | Low |
| F | Low | Medium | Low |

Step 4 Using the exposure and toxicity ranks, create a toxicity-exposure matrix for each medium.

TOXICITY-EXPOSURE MATRIX

| TOXICITY | AIR EXPOSURE | | | DRINKING WATER EXPOSURE | | | FISH INGESTION EXPOSURE | | |
|---|---|---|---|---|---|---|---|---|---|
| | LOW | MEDIUM | HIGH | LOW | MEDIUM | HIGH | LOW | MEDIUM | HIGH |
| LOW | B | | | | | B | | B | |
| MEDIUM | | D | C | C | D | | | C | D |
| HIGH | E,F | | A | E | F | A | A,E,F | | |

Step 5. Assign values to each cell in the matrix.

For this step, ranks are assigned the following values:

| Category | Exposure Rank | Toxicity Rank |
|---|---|---|
| High | 0.4 | 5 |
| Medium | 0.2 | 3 |
| Low | 0.1 | 1 |

The value for the cell is the product of the toxicity times the exposure rank.

TOXICITY-EXPOSURE MATRIX VALUES

| TOXICITY | AIR EXPOSURE | | | DRINKING WATER EXPOSURE | | | FISH INGESTION EXPOSURE | | |
|---|---|---|---|---|---|---|---|---|---|
| | LOW | MEDIUM | HIGH | LOW | MEDIUM | HIGH | LOW | MEDIUM | HIGH |
| LOW | 0.1 | | | | | 0.4 | | 0.2 | |
| MEDIUM | | 0.6 | 1.2 | 0.3 | 0.6 | | | 0.6 | 1 2 |
| HIGH | 0.5 | | 2 | 0.5 | 1 | 2 | 0.5 | | |

Step 6 Combine facility-specific emissions and population data to obtain media-specific chemical scores

EMISSION-EXPOSURE SCORES

(FOR AIR.)

| Facility | Chemical | Air Emissions (lb/yr) | Population Exposed via Air | Matrix Value | AIR SCORE |
|---|---|---|---|---|---|
| 1 | A | 1000 | 3000 | 2 | 6.0E+06 |
| | B | 2000 | 3000 | 0.1 | 6.0E+05 |
| | C | 2000 | 3000 | 1.2 | 7.2E+06 |
| | E | 4000 | 3000 | 0.5 | 6 0E+06 |
| 2 | C | 3000 | 1000 | 1.2 | 3.6E+06 |
| | D | 4000 | 1000 | 0.6 | 2.4E+06 |
| | F | 10000 | 1000 | 0.5 | 5.0E+06 |
| 3 | A | 2000 | 2000 | 2 | 8.0E+06 |
| | C | 4000 | 2000 | 1.2 | 9.6E+06 |
| | D | 6000 | 2000 | 0.6 | 7.2E+06 |
| | E | 1000 | 2000 | 0.5 | 1.0E+06 |
| | TOTAL: | | | | 5.7E+07 |

(FOR WATER):

| Facility | Chemical | Air Emissions (lb/yr) | Population Exposed via Water | Drinking Water Matrix Value | Fish Matrix Value | Average Matrix Value | WATER SCORE |
|---|---|---|---|---|---|---|---|
| 1 | A | 6000 | 500 | 2 | 0.5 | 1.3 | 3.8E+06 |
| | B | 4000 | 500 | 0.4 | 0.2 | 0.3 | 6.0E+05 |
| | C | 1000 | 500 | 0.3 | 0.6 | 0.5 | 2.3E+05 |
| | E | 3000 | 500 | 0.5 | 0.5 | 0.5 | 7.5E+05 |
| 2 | C | 1000 | 6000 | 0.3 | 0.6 | 0.5 | 2.7E+06 |
| | D | 5000 | 6000 | 0.6 | 1.2 | 0.9 | 2.7E+07 |
| | F | 2000 | 6000 | 1 | 0.5 | 0.8 | 9.0E+06 |
| 3 | A | 4000 | 2000 | 2 | 0.5 | 1.3 | 1.0E+07 |
| | C | 2000 | 2000 | 0.3 | 0.6 | 0.5 | 1.8E+06 |
| | D | 10000 | 2000 | 0.6 | 1.2 | 0.9 | 1.8E+07 |
| | E | 6000 | 2000 | 0.5 | 0.5 | 0.5 | 6.0E+06 |
| | TOTAL: | | | | | | 8.0E+07 |

Step 7 Combine the media-specific ranks to obtain overall rank.

| Facility | Chemical | AIR SCORE | WATER SCORE | OVERALL SCORE |
|---|---|---|---|---|
| 1 | A | 6.0E+06 | 3.8E+06 | 9.8E+06 |
| | B | 6.0E+05 | 6.0E+05 | 1.2E+06 |
| | C | 7.2E+06 | 2.3E+05 | 7.4E+06 |
| | E | 6.0E+06 | 7.5E+05 | 6.7E+06 |
| 2 | C | 3.6E+06 | 2.7E+06 | 6.3E+06 |
| | D | 2.4E+06 | 2.7E+07 | 2.9E+07 |
| | F | 5.0E+06 | 9.0E+06 | 1.4E+07 |
| 3 | A | 8.0E+06 | 1.0E+07 | 1.8E+07 |
| | C | 9.6E+06 | 1.8E+06 | 1.1E+07 |
| | D | 7.2E+06 | 1.8E+07 | 2.5E+07 |
| | E | 1.0E+06 | 6.0E+06 | 7.0E+06 |
| | TOTAL: | 5.7E+07 | 8.0E+07 | 1.4E+08 |

**Appendix B-a.**

# Briefing Paper
# Section 313, Title III
# Reporting Toxicity Information
# for Trade Secret Claimed Chemicals

USEPA
Office of Pesticides and Toxic Substances
Economics and Technology Division

# Briefing Paper
# Section 313, Title III
# Reporting Toxicity Information
# for Trade Secret Claimed Chemicals

## I. Introduction

Section 322 (h)(2) of Title III requires EPA to identify the adverse health and environmental effects associated with a section 313 chemical which is claimed trade secret under section 322 and assure that such information is included in the computer database. The legislative history associated with this provision further explains that the adverse effects identified should be described in general terms so as not to provide a unique identifier of a particular trade secret chemical.

EPA, in its final rule (40 CFR part 372 (IX)(B)), briefly discussed its approach to the problem of balancing trade secret protection versus providing adverse health and environmental effects information for section 313 chemicals. EPA developed a screening matrix of the 309 listed chemicals against the 10 health and environmental effects specifically mentioned in section 313. Toxicity data were gathered from selected information sources. The matrix was developed to aid in exploring various options for meeting the requirements claiming section 313 chemicals as trade secret. No detailed hazard assessment or literature evaluation was conducted during this exercise.

As described in the final rule, 70 chemicals exhibited unique toxicity patterns and thus, divulging such information would not protect trade secret claims. In its effort to adequately protect chemical identity when claimed trade secret, EPA began consolidating the toxicity categories in a sequential fashion until there were no unique patterns of toxicity for any of the 309 listed chemicals. The final result yielded only four general toxicity categories: carcinogenicity, acute toxicity, other human health effects, and environmental toxicity.

There are three other sections to this paper. Section II describes in detail the construction of the toxicity matrix and the health and environmental endpoints used to put an "X" in a box. Section III deals with the consolidation of the toxicity categories as described in the final rule as well as additional analyses done since that writing. Finally, section IV is a discussion of potential options based on the analyses in Section III. The Agency is seeking comments on the approach it used to attempt to balance trade secret provisions with disclosing of toxicity data as well as comments on the options presented in section IV.

## II. Background

### A. Construction of the Matrix

In an effort to analyze the possible options available under the constraints of section 322 of Title III, the Agency utilized the results of a limited screening exercise conducted by EPA in October 1986 to capture and describe the rationale used by New Jersey and Maryland in the development of their respective lists. Based on an analysis of this exercise, the Agency developed an expanded toxicity data matrix for the combined list of 329 chemicals and categories (EPA 1987). The matrix is intended to identify those adverse health and environmental effects that have been reported to be associated with each section 313 chemical. The health and environmental endpoints included in this matrix are limited to those specifically mentioned in section 313: carcinogenicity, heritable gene and chromosomal mutations, developmental toxicity (including teratogenicity), reproductive toxicity, acute toxicity, chronic toxicity, neurotoxicity, environmental toxicity, and persistence and bioaccumulation in the environment. Appendix A contains the toxicity matrix for the 309 listed section 313 chemicals. Appendix B contains the same toxicity matrix including the information sources used to identify data indicating potential human and environmental toxicity for each chemical.

The toxicity matrix is a summary presentation of information publicly available through a number of accessible databases: Hazardous Substances Databank (HSDB), RTECS, GENETOX, AQUIRE, ENVIROFATE, Log P database, and CHEMTRACK. Although the data from these sources have not been evaluated, the data serve the purpose of analyzing potential approaches for disseminating toxicity information for trade secret claimed chemicals. Endpoints for which available data suggest evidence that there may be a causal relationship between exposure and the observed toxicity are indicated with an "X" in the appropriate fields on the matrix. The absence of an "X" for a particular effect does not indicate that a chemical is known to be safe for the indicated effect. Rather, absence of an "X" indicates that either data to support a concern were not found in the database reviewed, or were not available at the time the matrix was constructed, or that the available data did not suggest sufficient evidence of potential toxicity. The source(s) of data from which each "X" is determined is documented so that it will be possible to alter the list if new data are identified, or if it is determined that any particular data source is inappropriate or inadequate.

It should be noted that this is only a screening exercise. The data sources used to construct the matrix were readily available but may not be the only sources used to construct a toxicity matrix. Validation of the data reported in the database sources has not been performed and some of the databases are not peer reviewed. An "X" indicates the availability of data relative to an effect; it does not indicate severity or validity

of concern.

B. Health and Environmental Endpoints

For the purposes of generating a toxicity matrix for section 313 chemicals, thresholds or limitations were established for the health and environmental endpoints evaluated. These thresholds or limitations were used to make rough determinations using the data within this limited search. Underlying studies were not collected, reviewed, or validated as the objective of this exercise is to determine which approach might best balance trade secret provisions and the dissemination of toxicity data in the database. It is also important to note that the matrix does not necessarily reflect Agency limitations and thresholds which would satisfy the listing and delisting of substances from section 313 reporting since each chemical would need to undergo a detailed hazard assessment.

1. Carcinogenicity

This category provides information on the known or potential human carcinogenicity of a chemical. For this endpoint, an "X" indicates that the available data support a concern for a chemical's carcinogenic potential if one or more of the following applied:

(a) A positive result was reported for that chemical in one or more animal species in an NCI or NTP bioassay;

(b) The IARC carcinogen classification for that chemical is human positive or human suspected and/or animal positive or animal suspected;

(c) The EPA carcinogen classification for that chemical is A (human carcinogen), B1 or B2 (probable human carcinogen), or C (potential human carcinogen; or

(d) the Gene-Tox carcinogen evaluation of that chemical is sufficient positive or limited positive evidence of carcinogenicity.

The NTP results and IARC, EPA, and Gene-tox classifications for each chemical are presented in the toxicity matrix (Appendix B) under the appropriate column heads. The carcinogen bioassay results and classifications were obtained from the following sources: CHEMTRACK (NTP evaluation, EPA classification), RTECS (IARC classification), and GENETOX (Gene-tox evaluation). The EPA, IARC, and Gene-tox classifications are based on weight-of-evidence in which the carcinogenic potential of a chemical is evaluated. The NTP evaluation is limited to the results of bioassays in experimental animals conducted by NTP and reflect whether a chemical was found to be positive or negative in the bioassay.

2. Heritable Genetic and Chromosomal Mutation

For this endpoint, an "X" indicates that the available data support concern that the chemical has the potential to produce heritable mutations in human germ cells. Valid positive results from studies on heritable mutation events (of any kind) in germ cells were sufficient evidence to indicate a potential positive response. In addition, evidence that an agent interacts with germ-cell DNA or other chromatin constituents or that it induces such endpoints such as unscheduled DNA synthesis, sister-chromatid exchange, or chromosomal aberrations in germinal cells was sufficient evidence to indicate a potential positive response. The criterion used to indicate a positive response for an agent was a positive result in one or more of the following bioassays as reported in the results table for each chemical in the GENETOX database:

(a) Drosophila melanogaster sex-linked recessive lethal test;

(b) Drosophila melanogaster heritable (reciprocal) translocation test;

(c) Mouse heritable translocation test;

(d) Drosophila melanogaster sex chromosome gain/loss (aneuploidy);

(e) Rodent dominant lethal test;

(f) Unscheduled DNA synthesis, sister-chromatid exchange, or chromosomal aberrations in germinal cells; and

(g) Mouse specific locus test (germ cells).

3. Developmental Toxicity

For this endpoint, an "X" indicates that the available data support concern that the chemical cause developmental toxicity in humans. Developmental toxicity is any detrimental effect produced by exposures to developing organisms during embryonic stages of development and includes embryotoxicity, fetotoxicity, and teratogenicity. The major manifestations of developmental toxicity include: (1) prenatal or early postnatal death; (2) structural abnormalities; (3) altered growth (usually in the form of growth retardation); and (4) functional deficits which may include reduced pulmonary function, reduced immunological competence, neurobehavioral deficits such as learning disorders or mental retardation, etc. The exposure period may be prior to conception (either parent), during prenatal development, or postnatally to the time of sexual maturation. Developmental effects, however, may be detected at any time in the lifespan of the organism.

An "X" is indicated for a chemical if the available data provide evidence that the chemical produces developmental toxicity at body doses of less than or equal to 1 g/kg/day. HSDB was examined for data on the developmental toxicity of a chemical following inhalation, oral, or dermal exposure. When necessary, exposure doses were converted to body doses using the reference value for body weight, inhalation rate, water consumption, and food factors for each species recommended by EPA (1985).

4. Reproductive Toxicity

For this endpoint, an "X" indicates that the available data support concern that the chemical causes adverse effects on male or female reproductive performance. Endpoints of concern include, but are not limited to, effects on gonadal function, estrous cycle, mating behavior, conception, parturition, lactation, and weaning.

An "X" is indicated for a chemical if the available data provide evidence that the chemical causes reproductive dysfunction or reproduction damage at body doses less than or equal to 1 g/kg/day. HSDB was examined for data on the reproductive toxicity of an agent following inhalation, oral or dermal exposure. When necessary, exposure doses were converted to body doses using the reference values for body weight, inhalation rate, water consumption, and food factors for each species recommended by EPA (1985).

5. Acute Toxicity

For this endpoint, an "X" indicates that the available data support concern that short-term exposure, at or below a specified level, to the chemical by the inhalation, oral, or dermal route has been determined to cause death in 50% of the exposed test population.

An "X" is indicated for a chemical if the available data provide evidence that the reported median of the lethal concentration ($LC_{50}$) for the chemical following inhalation exposures for 8 hours or less was less than or equal to 5 mg/liter (5,000 $mg/m^3$); the reported median of the lethal dose ($LD_{50}$) for the chemical following oral exposure was less than or equal to 250 mg/kg; or the $LD_{50}$ for the chemical following dermal exposure was less than or equal to 500 mg/kg. RTECS was examined for data on the acute toxicity of chemicals in mammals following short-term inhalation, oral, or dermal exposure. When necessary, doses expressed in ppm were converted to $mg/m^3$ using the ideal gas law (PV=nRT).

6. Chronic Toxicity

Chronic effects for the purposes of Section 313 reporting are any adverse effects other than cancer observed in humans or animals resulting from long-term exposure to a chemical. In

chronic toxicity studies, animals are usually exposed to a test chemical by inhalation, dermal, or oral routes for more than 90 days. Thus the observed adverse effects are due to continuous or frequently recurring insult of target organs with relatively small doses or low concentrations for a prolonged period of time.

An "X" is indicated for an agent if the available data provide evidence that the chemical produces adverse health effects at body doses of less than or equal to 1 g/kg/day following inhalation, oral, or dermal exposure for more than 90 days. HSDB was examined for data on the chronic toxicity of a chemical. When necessary, exposure doses were converted to body doses using the reference values for body weight, inhalation rate, water consumption, and food factors for each species recommended by EPA (1985).

7. Neurotoxicity

Neurotoxicity is any adverse effect on the structure or function of the central and/or peripheral nervous system related to exposure to a chemical substance. Neurotoxic effects may be morphological (neuropathological effects, biochemical changes) or functional (behavioral, electrophysiological, or neurochemical effects).

An "X" is indicated for an agent if the available data provide evidence that chronic (at least 90-days) inhalation, oral, or dermal exposure to the chemical is reported to result in morphological or functional neurotoxic effects at body doses of less than or equal to 1 g/kg/day. Reported biochemical changes in the absence of functional or histopathological effects was not considered an adequate basis for listing a chemical. HSDB was examined for data on the neurotoxicity of an agent following long-term exposure. When necessary, exposure doses were converted to body doses using the reference values for body weight, inhalation rate, water consumption, and food factors for each species recommended by EPA (1985).

8. Environmental Toxicity

Section 313 of SARA allows the Agency to add a chemical to the Emissions Inventory if it is known to cause or can reasonably be anticipated to cause a serious, significant adverse effect on the environment. The judgement may be based on toxicity alone or toxicity and a consideration of either persistence in the environment or tendency to bioaccumulate in the environment. The toxicity matrix reflects a screening of information on the acute toxicity, bioaccumulation, and persistence of an agent. An $LC_{50}$ value of less than or equal to 100 ppm was considered to suggest sufficient evidence that a chemical is a potential environmental toxicant. For aquatic species, an "X" is indicated for a chemical based on environmental toxicity if the available data provide evidence that the reported $LC_{50}$ for that chemical for

less than or equal to 96 hours is less than or equal to 100 ppm; if the reported $LC_{50}$ for a chemical is less than or equal to 100 ppm and the chemical has a half-life of greater than or equal to 4 days; or if the reported $LC_{50}$ for a chemical is less than or equal to 100 ppm and the chemical has a log bioconcentration factor greater than or equal to 3, a measured log P of greater than or equal to 4.35, or an estimated log P of greater than or equal to 5.5.

The environmental toxicity column that indicates $LC_{50}$ values of less than or equal to 10 ppm is included in the matrix because chemicals that are reported to have $LC_{50}$ values of less than or equal to 10 ppm are of greater concern as potential toxicants, and this information may be used to set priorities for further review. The data in this column are not included in the algorithm analysis. The data for environmental toxicity were obtained from the following databases: AQUIRE (acute aquatic toxicity), ENVIROFATE (bioconcentration factors, half-lives, and measured log P values). AQUIRE contains reviews of aquatic toxicity studies and ranks the reliability of each study on a scale of 1 to 4. A study reliability of 1 indicates that the study is reliable, reliability 2 indicates that the study is generally satisfactory, reliability 3 indicates that study is not reliable, and reliability 4 indicates that the AQUIRE entry is a review of a study abstract or summary from a foreign paper. The reliability of the data obtained from AQUIRE used to determine an "X" for an environmental toxicant is documented on the matrix; when possible, the most reliable data were used to determine an "X".

# Appendix C

## Available Toxicity Data for TRI Chemicals

This appendix provides a summary of available toxicity data for the TRI chemicals. The data entered into the tables in this appendix were obtained primarily from EPA documents and were supplemented with relevant data from other sources. Citations are listed in the tables for all values. There are five major types of data provided: reportable quantities (RQs), reference doses, cancer potencies, ecological criteria, and other toxicological data. Each type of data and its major sources is discussed briefly below. The data sources are listed at the end of this section.

## REPORTABLE QUANTITIES

The RQ values were obtained primarily from the Technical Background Documents to Support Rulemaking Pursuant for CERCLA Section 103, Volumes 1 through 3 (March 1985 to July 1989). In some cases, the information was obtained from other sources and the sources are cited in the table.

## REFERENCE DOSES

The reference dose data were obtained from a number of sources. Only one value is provided for each exposure route per chemical. The hierarchy for selection of the most appropriate reference dose data was as follows: IRIS, HEAST, data from a Health and Environmental Review Division (HERD) evaluation of TRI chemicals, RQ support documents, and data from the Office of Pesticide Programs (OPP). The hierarchy is based on the level of review which the values received. Values listed on IRIS data base receive Agency-wide review and are developed using an Agency-wide assessment protocol. The values in the HEAST tables are also widely reviewed, but contain some values from a table identified as Alternate Methods. The HERD values are the result of a review of available literature for certain TRI chemicals. This review was conducted by OPPT scientists. Reference doses obtained from RQ documents were generated to support the RQ quantities and provide only brief descriptions of the toxicity evaluations carried out to generate the values. These are reviewed within the agency and, in many cases, are reviewed by interested parties in the private sector. OPP values are generated by the Office of Pesticide Programs for pesticides, based on pesticide registration data and other literature sources.

## CANCER POTENCIES

The selection of cancer potency values followed the hierarchy outlined for reference doses. In addition, a recently completed list of cancer potencies developed by the Office of Environmental Health Hazard Assessment in California's Environmental Protection Agency was consulted to obtain cancer potencies for 22 chemicals which appeared on the California list but were unavailable from EPA (CEPA, 1992).

## ECOLOGICAL CRITERIA

Values for the protection of aquatic life were obtained from the EPA's ambient water quality criteria. These values are published by EPA's Office of Water.

## OTHER TOXICOLOGICAL DATA

Reference doses and cancer potencies were not available from EPA for a number of chemicals on TRI. Consequently, other sources of information were consulted to determine if sufficient data were available to develop reference doses and cancer potencies for chemicals currently lacking values. Individual data searches for toxicological and epidemiological data for each chemical were beyond the current scope of this project. However, data bases such as the Hazardous Substances Data Base (HSDB) and the Registry of Toxic Effects of Chemical Substances (RTECS) provide succinct summaries of toxic effects and quantitative data, toxicological and epidemiological studies, and, in some cases, regulatory and carcinogenic status data.

The two data bases differ in both the type of presentation and the scope of the resources from which they obtain data. HSDB provides a brief discussion of most studies and results. It contains physical, ecological and toxicological data for most chemicals included in the data base. RTECS includes a greater number of chemicals and incorporates information from a wider array of sources. However, the data summaries are very brief, cryptic and only toxicological and epidemiological data are provided. HSDB generally contains fewer citations than RTECS because the literature contained in HSDB is limited to that which has been reviewed and found acceptable by EPA. However, HSDB often provides more detailed information on the studies than RTECS.

HSDB on line searches have been carried out for all chemicals under evaluation in this report which lack reference dose, cancer potency, or RQ data. All relevant categories of information were obtained for each chemical. An example of an HSDB printout is provided at the end of this section for 1,4-benzoquinone.

The data bases do not provide a sufficient level of detail to choose the best studies or calculate reference doses or cancer potencies. However, they can be used to identify those chemicals for which dose-response data are available and to obtain citations. In addition to HSDB and RTECS, other data bases such as the International Register of Potentially Toxic Chemicals (IRPTC), and literature searches may be useful in identifying relevant dose-response data for development of health risk values.

If dose-response data were obtained for TRI chemicals currently lacking reference dose and cancer potency values, the values could be calculated using standard EPA assessment methodology. The following discussion outlines standard methods used to calculate reference doses and cancer potencies utilizing dose-response data.

## Reference Doses

Reference doses are calculated for non-carcinogens. It is assumed that for non-carcinogens and non-mutagens, a threshold exists below which exposure does not cause adverse health effects (EPA, 1988). Thresholds for the effects of chronic exposure are estimated from the No Observable Adverse Effects Level (NOAEL) or Lowest Observable Adverse Effects Level (LOAEL) obtained from toxicological studies of animals and humans or epidemiological studies of humans. To account for the various types of uncertainty inherent in estimating a threshold for health effects, Uncertainty Factors and Modifying Factors are utilized. These are based on specific characteristics of the toxicological data, and are summarized in Figure C-1. The Uncertainty and Modifying Factors are divided into the NOAEL or LOAEL to obtain a reference dose which is an estimated safe exposure level for the general population. This approach parallels EPA's methodology for derivation of RfDs. However, an in-depth analysis of the epidemiological and toxicological literature is conducted by EPA when developing its risk values.

### Methods

Reference doses can be calculated for specific routes of exposure. They are generally referred to as reference concentrations (RfCs) for inhalation exposure. There are 3 steps to calculate an RfC:

1. identify the most appropriate NOAEL or LOAEL

2. apply relevant Uncertainty Factors and Modifying Factors

3. calculate media specific reference doses

### 1. Identify the Most Appropriate NOAEL or LOAEL.

The hierarchy used to select a NOAEL or LOAEL is as follows:

- a human study is preferable to an animal study, when a human study is unavailable an animal study using the most sensitive species for the toxic effect of concern is preferable

- chronic (lifetime) study is preferable to a subchronic study (an acute study cannot be used to quantify risks associated with chronic exposure

- a study with the appropriate exposure route(s) is preferable: oral or gavage for oral exposure and inhalation for airborne exposure)

- a study with sufficient subjects to obtain statistical significance at relatively low exposure levels is required

FIGURE C-1. UNCERTAINTY FACTORS AND MODIFYING FACTORS

| NUMERICAL VALUE | REASONING |
|---|---|
| **UNCERTAINTY FACTORS** | |
| 10 | INTERSPECIES: accounts for variation in sensitivity among population members |
| 10 | INTRASPECIES: accounts for uncertainty in extrapolating from animals to humans |
| 10 | SUBCHRONIC DATA: accounts for uncertainty arising from extrapolation of less than a lifetime study (subchronic) to a lifetime exposure (chronic) |
| 10 | LOAEL: accounts for uncertainty resulting from the use of data which demonstrated an adverse effect, to estimate a level at which no effect is expected to occur |
| **MODIFYING FACTOR** | |
| 0 - 10 | QUALITY OF DATA: based on scientific uncertainties not explicitly treated in the Uncertainty Factors such as the completeness of the data base, concordance of results, number of species tested, etc. The default value is 1. |

(adapted from 1.2.2.2.4 in EPA, 1988)

- a recent study identifying adequately sensitive endpoints is required (e.g. not mortality)

- an adequate control population is required

- in general, a NOAEL is preferable to a LOAEL. Usually, the LOAEL which generates the lowest exposure threshold (after the application of Uncertainty and Modifying Factors) is selected.

Issues related to the quality of the study should also be considered in selecting the most appropriate studies. Additional information on selection criteria can be reviewed in the IRIS documentation file (EPA, 1988).

2. Apply Relevant Uncertainty and Modifying Factors.

Using the information in Figure C-1, factors are applied which depended on the characteristics of the study and the NOAEL or LOAEL, e.g. 10 for an animal study, 10 for a subchronic study. The NOAEL or LOAEL is divided by the factors to obtain a reference dose in mg/kg-day.

EXAMPLE: chemical X has a NOAEL of 5 mg/kg-day, based on a subchronic study in mice fed chemical X in their diet.

Uncertainty factors of 10 for intraspecies, 10 for interspecies, and 10 for the subchronic nature of the study are divided into the NOAEL:

$$RfD = \frac{5 \text{mg/kg-day}}{10 \times 10 \times 10} = 0.005 \text{ mg/kg-day}$$

3. Calculate Media Specific Reference Doses

The reference dose in mg/kg-day is used derive a media-specific reference dose. For waterborne contaminants the concentration per liter of water is used; for airborne contaminants the concentration per cubic meter of air is used. It is assumed that the average water consumption in the general population is 2 liters per day and that the average air intake volume is 20 $m^3$ per day. It is assumed that the average body weight of humans is 70 kg. The RfD in mg/kg-day is used with these values to obtain a threshold in air or water. It is recognized that these average values do not apply to all individuals; however,

for purposes of developing TRI indices, some generalizing assumptions are used. To obtain units comparable to EPA's air and water guidelines, the reference dose units were converted to ug from mg through multiplying by 1000.

EXAMPLE: chemical X (above) has no RfD or RfC; therefore both airborne and waterborne exposure thresholds must be estimated.

WATERBORNE EXPOSURE

$$\frac{0.005 \text{ mg/kg-day} \times 70 \text{ kg} \times 1000 \text{ ug/mg}}{2 \text{ liters/day}} = 175 \text{ ug/liter}$$

AIRBORNE EXPOSURE

$$\frac{0.005 \text{ mg/kg-day} \times 70 \text{ kg} \times 1000 \text{ ug/mg}}{20 \text{ m}^3\text{/day}} = 1.75 \text{ ug/m}^3$$

The absorption and metabolism of chemicals, and, in some cases, the health effects observed, frequently differ between routes of exposure. EPA suggests that utilization of a study which does not have the appropriate route of exposure contributes to the overall uncertainty of the risk value. Using the simplified approach taken in this work, it will not be possible to fully evaluate the route-specific differences in response to the chemicals unless NOAELs or LOAELS exist for both routes. In this case, individual reference doses are calculated for each route.

## Carcinogens

EPA and most risk assessors take a probabilistic approach to estimating carcinogenic risks based on the general assumption that any exposure to a carcinogen will generate some cancer risk. Consequently, carcinogens are not considered to have a safe threshold for exposure. The risk is proportional to the cumulative exposure, and at low exposure levels may be very small. Carcinogenic risk is usually expressed as a slope factor or $q_1^*$ value with units of risk per mg/kg-day. Risk may also be estimated for specific media. When risks in

air and water are provided these are referred to as unit risks because they are expressed per unit of air or water.

EPA utilizes various methods to estimate carcinogenic risk for individuals and populations. For most chemicals, it is necessary to estimate risks at low exposures from data which is obtained from high exposure studies. The required extrapolation may be carried out using a variety of models. Generally EPA uses a linearized multistage model, in the absence of information requiring other approaches (51 FR (185) 33997). The use of this model generates a plausible upper limit risk estimate. The multistage model has the general form:

$$P(d) = 1 - \exp - (q_0 + q_1 d + q_2 d^2 + \ldots + q_k d^k)$$

where:

d = dose
P(d) = the lifetime risk of cancer at dose d

Epidemiological and toxicological dose-response data are used to provide the dose and probability inputs to the model. A upper bound estimate of response is calculated and a modification to equalize doses between species is applied when non-human studies are used. Unless a large amount of dose-response data is available, the $q_1$ value is often the only data point obtained from the equation. This is usually referred to as the cancer potency or slope factor and estimates upper bound risk per mg/kg-day. The methods used to estimate cancer risk are discussed in detail in the IRIS documentation (EPA, 1988) and EPA"s "Guidelines for Cancer Risk Assessment (51 FR (185) 33992-34003 (9/24/86)). This model does not necessarily provide a realistic risk prediction. Rather, it provides an upper estimate of risk. The actual risk may be significantly lower.

Methods

Cancer potencies may be calculated for both oral and inhalation exposure. There are 4 major steps to calculate cancer potency.

1. identify most appropriate dose response data

2. modify dose data for interspecies differences

3. calculate the 99% upper confidence bound on the data

4. develop an equation describing the dose response relationship

1. Identify the Most Appropriate Dose Response Data.

Various criteria are used to select appropriate dose response data for carcinogenic risk estimates. In some cases, data from a number of studies can be aggregated. However, due to interspecies differences this is usually only done for multiple human data sets. The criteria generally applied are:

- human data are preferable to animal data
- animal data from species whose biological responses are most like those of humans are preferable
- in the absence of the previous two, data from the most sensitive species are preferred
- the route of exposure resembling that being evaluated in humans is preferred
- tumors at more than one site are used to identify all animals with tumors
- benign tumors with the potential to progress to malignant tumors of the same histogenic origin are combined with malignant tumors to quantify tumor incidence
- consistency in response among studies provides qualitative support for the results

The criteria for selection of appropriate data is discussed in the IRIS documentation (EPA, 1988).

2. Modify Dose Data for Interspecies Differences.

When the dose response data is not obtained from a human study, it is necessary to make adjustments to the dose to account for differences between animals and humans in their body weight and surface area ratios. Surface area is thought to be more closely related to response than body weight. Therefore, using only body weight will not provide the most accurate estimate of predicted responses. Surface area can be approximated by body weight to the 2/3 power. The adjustment is carried out by raising the body weight of both the animal and of humans (assumed to be 70 kg) to the 2/3 power, and using the resulting ratio to estimate an equivalent human dose. EPA recommends using a factor of 13 for mice and 5.8 for rats in dose adjustments (e.g. the dose is divided by 13 to provide a human equivalent), which is based on standard weights for the animals (EPA, 1988).

EXAMPLE: a lifetime study of male mice with an average adult weight of .03 kg yielded 10 malignant tumors in 50 animals dosed orally with chemical X at 50 mg/kg-day and no tumors in 50 control animals.

$$\frac{50 \text{ mg/kg-day}}{13} = 3.85 \text{ equivalent human dose}$$

3. Calculate an Upper 99% Confidence Bound on the Data.

Confidence bounds are related to the reliability of the data as determined by sample size. With a large number of study subjects the confidence in the study results will be high and the confidence bounds around the actual observed responses will be relatively small. With a small number of subjects the reverse will be true.[1] A Poisson distribution can be used to estimate the binomial distribution and obtain a 99% confidence bound. The Poisson distribution (Pearson and Hartley, 1966) can be used in cases where the observed responses affect 20% or fewer of the study subjects and the population size is at least 50. More information on confidence bounds and equations which can be used to calculate confidence bounds are found in any basic statistics book. The upper bound value can be converted to a ratio using the relationship:

$$\text{upper bound response value} = \frac{\text{99\% upper bound on number responding}}{\text{number of subjects in exposure group.}}$$

This provides a single value representing the upper bound on response for that exposure group.

EXAMPLE: (using the data provided in step 2 above) 10 of the 50 animals developed tumors. Using the Poisson Distribution the upper 99% limit on 10 is 20.[2]

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[1] Tests of significance will not be discussed here because it is assumed that the data used for these analyses have met tests of significance as a requirement of its incorporation into the data bases.

[2] This example shows a control group with 0 responses. The approach becomes more complex in cases where the control group has respondents. Methods used to adjust for background responses in the control group are provided in toxicology and epidemiology texts.

The upper 99% confidence bound response value is 20. Thus the ratio is:

$$20/50 = 0.4$$

This indicates that there is a 99% chance that the value of 0.4 would not be exceeded if the same experiment were repeated numerous times. The 99% upper confidence bound value is used as the response data in the development of the linear equation which describes the dose response relationship.

4. Develop an Equation Describing the Dose Response Relationship.

A simple linear equation of the form $y = ax$ is calculated from the upper bound dose response data. The equation is derived from the lowest dose data point available from the chosen study and the 0 dose and 0 response data point is obtained using the algebraic equation for a line between two points:

$$a = \frac{y(2) - y(1)}{x(2) - x(1)}$$

where:

x(1) is the 0 dose
y(1) is the 0 response
x(2) is the study dose
y(2) is the 99% upper confidence bound study response

EXAMPLE: using the data obtained in step 3 above, the input to the equation is:

x(1) = 0
y(1) = 0
x(2) = 0.005
y(2) = 0.4

Using these in the equation above yields:

$$a = \frac{0.4 - 0}{0.005 - 0} = 80$$

The resulting equation is: $y = 80x$.

In cases where dose-response information is available in the exposure range of the general population (at very low doses), the actual dose response data can be used without extrapolation to develop an equation describing the dose response relationship. This can be done using regression analysis (linear, exponential or power regression) and requires only a hand-held calculator. The assumption that the equation continues through the 0 dose, 0 response data point is included in the data input into the equation. Sufficient data for this type of analysis is usually available only if exposure of the general population has occurred which would generate exposure at very low doses. The results of this type of analysis may generate a much more accurate evaluation of risk, because actual responses have been measured in the range at which the population is exposed.

## REFERENCES

CEPA (California Environmental Protection Agency). 1992. "Expedited Cancer Potency Values and Proposed Regulatory Levels for Certain Proposition 65 Carcinogens." Office of Environmental Health Hazard Assessment, Reproductive and Cancer Hazard Assessment Section. April.

Hazardous Substances Data Base. 1992. Available on-line from Toxnet. Retrievals performed September, 1992.

Pearson and Hartley, eds. 1966. Biometrika Tables for Statisticians, Vol.1. Cambridge University Press.

U.S. Department of Health and Human Services, NIOSH. 1992. Registry of Toxic Effects of Chemical Substances (RTECS). Available on-line through Toxnet.

U.S. Environmental Protection Agency (EPA). 1988. Integrated Risk Information System (IRIS), Background Document I. Washington, D.C. February 10.

THE FOLLOWING HSDB CHEMICAL FILE WAS OBTAINED THROUGH TOXNET

SEPTEMBER, 1992

AME - 1,4-BENZOQUINONE
N - 106-51-4
TOXS - NO DATA
TXHR - Classification of carcinogenicity: 1) evidence in humans: No data; 2) evidence in animals: Inadequate. Overall summary evaluation of carcinogenic risk to humans is Group 3: The agent is not classifiable as to its carcinogenicity to humans. /From table/ [IARC MONOGRAPHS. 1972-PRESENT S7 71 (1987)] **PEER REVIEWED**

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THE FOLLOWING OVERVIEW IS A SUMMARY. CONSULT THE COMPLETE POISINDEX (R) DATABASE FOR TREATMENT PURPOSES. COPYRIGHT 1974-YEAR MICROMEDEX, INC. ALL RIGHTS RESERVED. DUPLICATION PROHIBITED.

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EMT -

o EMLS - LIFE SUPPORT :

This overview assumes that basic life support measures have been instituted.

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o EMCE - CLINICAL EFFECTS :

SUMMARY

- Acute ingestions of hydroquinone up to 500 mg/day for 5 months produced no symptoms in man. Oral quinone poisoning has not been reported in man.

HEENT

- Both hydroquinone and quinone are known to cause eye irritation from chronic dust or vapor exposure. Keratitis, corneal ulceration, and discoloration of the conjunctiva may occur.

CARDIOVASCULAR

- Pallor, cyanosis, and C-V collapse were reported.

RESPIRATORY

- Lung irritation is possible with chronic exposures to vapors or dust. Ingestion has caused dyspnea, anoxia, and respiratory failure.

NEUROLOGIC

- Dizziness, headache and delirium have been reported with hydroquinone.

GASTROINTESTINAL

- Vomiting and GI irritation have been seen.

HEPATIC

- Nonspecific liver changes and jaundice have been reported. Nonspecific hematologic effects have been seen in animals.

DERMATOLOGIC

- Dermatitis, hypomelanosis and delayed hyperpigmentation have occurred.

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o EMLAB- LABORATORY :

- Hydroquinone is not found naturally in the body. A urine screen which detects hydroquinone is indicative of exposure. Hydroquinone may turn the urine green or brown-green.

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o EMTR - TREATMENT OVERVIEW :

SUMMARY

- Acute hydroquinone-quinone exposures are rare and experience is limited. Available data indicates symptoms and treatment should be similar to phenol.

ORAL EXPOSURE

- Although not as irritating as phenol, dilution with

water or milk is indicated.
INHALATION EXPOSURE
EYE EXPOSURE
DERMAL EXPOSURE

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o EMTOX- RANGE OF TOXICITY :

- o Acute ingestions of hydroquinone up to 500 mg/day for 5 months produced no symptoms. 1 gm of hydroquinone in an adult has caused symptoms, and death has occurred with 5 gm.

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o REFERENCE : [Rumack BH & Spoerke DG: POISINDEX(R) Information System. Micromedex Inc., Denver, CO, 1990; CCIS CD-ROM Volume 68, edition exp May, 1991. ] .**PEER REVIEWED**

ANTR - NO DATA

MEDS - Careful examination of eyes, incl visual acuity & slit lamp examinations, should be done during placement & periodic examinations. Also evaluate skin. [SITTIG. HANDBOOK TOXIC HAZARD CHEM & CARCINOG 2 ED 85 , p. 765] **PEER REVIEWED**

HTOX - ULCERATION OF CORNEA HAS RESULTED FROM ONE BRIEF EXPOSURE TO HIGH CONCN OF VAPOR OF QUINONE, AS WELL AS FROM REPEATED EXPOSURES TO MODERATELY HIGH CONCN. FOLLOWING DISCONTINUATION OF EXPOSURE, RECOVERY OCCURRED PROMPTLY & SPONTANEOUSLY ... THERE WERE NO SYSTEMIC EFFECTS OR CHANGES IN COMPOSITION OF BLOOD OR URINE. [PATTY. INDUS HYG & TOX 3RD ED VOL2A,2B,2C 1981-82 , p. 2594] **PEER REVIEWED**

HTOX - CAN CAUSE DERMATITIS WITH DISCOLORATION, ERYTHEMA, FORMATION OF PAPULES & VESICLES. IN SEVERE CASES THERE CAN BE NECROTIC CHANGES IN SKIN. VAPORS ACTING ON EYE CAN CAUSE SERIOUS DISTURBANCES, INCL CONJUNCTIVITIS ... DISCOLORATION OF CONJUNCTIVA & CORNEA HAVE BEEN REPORTED. [MERCK INDEX. 10TH ED 1983 , p. 1168] **PEER REVIEWED**

HTOX - ... Ocular disturbance without acute reaction was observed in numerous workers who were exposed chronically to vapors of benzoquinone or dust of hydroquinone. These workers developed in course of 2 years a brownish tinge overlying the sclera in the palpebral fissure. At this stage, the conjunctival surface appeared slightly dry, & deeper layers of conjunctiva had a light brownish stain visible biomicroscopically, but no discrete colored particles. After another 2 or 3 years, the conjunctiva appeared more thickened & more dry, with superficial white flecks & brown stain. In deeper layers, brown discoloration was ... seen ... as discrete brown granules or globules. Pigment was observed to begin to migrate from limbus into cornea. [GRANT. TOX OF THE EYE 1986 , p. 498] **PEER REVIEWED**

HTOX - ... In several cases /of chronic exposure to quinone/ vision became seriously reduced from permanent fine opacities & much astigmatism & irregularity in the cornea. After exposure to quinone vapor was discontinued, the discoloration decreased, but the visual disturbance was permanent. Many years later in such cases a Hudson-Stahli pigment line in the epithelium & severe astigmatism from formation of facets in cornea have been observed. [GRANT. TOX OF THE EYE 1986 , p. 498] **PEER REVIEWED**

HTOX - Target organs: Eyes, skin. Symptoms: Conjunctival keratitis; ulceration of skin. [NIOSH. NIOSH POCKET GUIDE CHEM HAZ 2ND PRT 1987 , p. 203] **PEER REVIEWED**

HTOX - IN MANY INDUSTRIES FINE DUST OF PARTICLES CAN BE GENERATED ... & REACH THE EYE. ... /THE/ COLORLESS HYDROQUINONE DUST ... IS STORED IN LARGE GRANULES IN OR NEAR BASAL LAYER OF CORNEAL EPITHELIUM & IN SMALLER GRANULES IN THE MORE SUPERFICIAL EPITHELIUM. IT IS VISIBLE AS A BROWN BAND KERATOPATHY. [CASARETT AND DOULL'S TOXICOLOGY 3RD ED 1986 , p. 483] **PEER REVIEWED**

NTOX - A GROUP OF MICE WERE PAINTED WITH A 0.25% SOLN OF P-QUINONE IN BENZENE EVERY 1 OR 2 DAYS. OF 44 MICE THAT SURVIVED MORE THAN 200 DAYS, 3 DEVELOPED SKIN PAPILLOMAS, 1 DEVELOPED A SKIN CARCINOMA & 5 DEVELOPED

LUNG ADENOCARCINOMAS. WHEN 0.1% SOLN WAS USED, 41 MICE SURVIVED MORE THAN 200 DAYS, & 6 DEVELOPED SKIN PAPILLOMAS, 2 DEVELOPED SKIN CARCINOMAS & 10 DEVELOPED LUNG ADENOCARCINOMAS ($P < 0.05$). OF 46 SURVIVING CONTROLS TREATED WITH BENZENE, 1 DEVELOPED SKIN PAPILLOMA, & 2 DEVELOPED LUNG ADENOCARCINOMAS (TAKIZAWA, 1940) (THE WORKING GROUP NOTED THAT THE SEX & STRAIN OF ANIMALS & DURATION OF EXPT WERE NOT SPECIFIED). [IARC MONOGRAPHS. 1972-PRESENT V15 258 (1977)] **PEER REVIEWED**

NTOX - GROUP OF 25 MICE (SEX & STRAIN UNSPECIFIED) WERE EXPOSED /BY INHALATION/ TO 5 MG PARA-QUINONE IN 130 L CHAMBER FOR 1 HR, 6 TIMES/WK; 25 MICE WERE UNTREATED ... . IN 11 TREATED MICE THAT SURVIVED MORE THAN 100 DAYS, 2 LUNG ADENOCARCINOMAS WERE OBSERVED. AMONG 12 CONTROLS THAT DIED AFTER MORE THAN 100 DAYS, 2 LUNG ADENOMAS WERE OBSERVED (KISHIZAWA, 1954). IN ANOTHER EXPT CARRIED OUT UNDER SAME CONDITIONS OF EXPOSURE, 2 LUNG ADENOCARCINOMAS WERE FOUND IN 25 TREATED MICE, COMPARED WITH 1 LUNG ADENOMA AMONG 25 CONTROLS (KISHIZAWA, 1955). THE SAME EXPT WAS REPEATED & 2 LUNG ADENOCARCINOMAS WERE OBSERVED IN 25 MICE & 1 LUNG ADENOMA IN 25 CONTROLS (KISHIZAWA, 1956). [IARC MONOGRAPHS. 1972-PRESENT V15 259 (1977)] **PEER REVIEWED**

NTOX - A GROUP OF 24 RATS (15 WISTAR STRAIN & 9 HYBRIDS), WEIGHING ABOUT 200 G EACH, WERE INJECTED SC WITH 0.5 ML SOLN OF P-QUINONE IN PROPYLENE GLYCOL AT WEEKLY INTERVALS. CONCN GIVEN DURING THE FIRST 53 DAYS WAS 1%; THIS WAS REDUCED TO 0.2% FROM DAYS 54-173 & AGAIN INCREASED TO 0.4% AFTER 173 DAYS. 17 RATS SURVIVED THE INJECTION PERIOD OF 394 DAYS & RECEIVED A TOTAL OF 32 INJECTIONS (P-QUINONE 81 MG, PROPYLENE GLYCOL 16.5 ML) DURING THIS PERIOD. INJECTION SITE FIBROSARCOMAS DEVELOPED IN 2 RATS. NO LOCAL TUMORS WERE OBSERVED AMONG 11 RATS OF SAITAMA MIXED STRAIN INJECTED WEEKLY WITH 1 ML PROPYLENE GLYCOL FOR 15 MO, THEN 0.5 ML, & SURVIVING 300 OR MORE DAYS ($P > 0.05$) (UMEDA, 1957). [IARC MONOGRAPHS. 1972-PRESENT V15 259 (1977)] **PEER REVIEWED**

NTOX - ASPHYXIA APPEARS TO PLAY IMPORTANT ROLE IN TERMINAL /CASES/ ... BECAUSE OF PULMONARY DAMAGE RESULTING FROM EXCRETION OF QUINONE INTO ALVEOLI & BECAUSE OF CERTAIN NOT TOO WELL-DEFINED EFFECTS OF QUINONE UPON HEMOGLOBIN. URINE OF SEVERELY POISONED ANIMALS MAY CONTAIN PROTEIN, BLOOD /&/ CASTS ... . [PATTY. INDUS HYG & TOX 3RD ED VOL2A,2B,2C 1981-82 , p. 2593] **PEER REVIEWED**

NTOX - ABSORPTION OF LARGE DOSES OF QUINONE FROM GASTROENTERIC TRACT OR FROM SC TISSUES OF ANIMALS INDUCED LOCAL CHANGES, CRYING, CLONIC CONVULSIONS, RESPIRATORY DIFFICULTIES, DROP OF BLOOD PRESSURE, & DEATH BY PARALYSIS OF MEDULLARY CENTERS. [PATTY. INDUS HYG & TOX 3RD ED VOL2A,2B,2C 1981-82 , p. 2593] **PEER REVIEWED**

NTOX - SIGNS OF KIDNEY DAMAGE WERE OBSERVED IN SEVERELY POISONED ANIMALS. ... IT ALSO CAUSES LOCAL GREYING OF HAIR OF COLORED MICE. [IARC MONOGRAPHS. 1972-PRESENT V15 259 (1977)] **PEER REVIEWED**

NTOX - TOXIC CONCN OF PARA-QUINONE WERE NOT MUTAGENIC TO NEUROSPORA TESTED FOR FORWARD PYR MUTATIONS (REQUIREMENT FOR PYRIMIDINES) OR REVERSE MUTATIONS TO ARGININE INDEPENDENCE. SINGLE IP INJECTION OF 6.25 MG/KG BODY WT PARA-QUINONE DID NOT INDUCE DOMINANT LETHAL MUTATIONS IN MALE MICE. [IARC MONOGRAPHS. 1972-PRESENT V15 260 (1977)] **PEER REVIEWED**

NTOX - THE BEHAVIORAL SYMPTOMS OF ACUTE P-BENZOQUINONE INTOXICATION IN THE COCKROACH (PERIPLANETA AMERICANA) WERE INITIAL EXCITATION FOLLOWED BY RIGID PARALYSIS. P-BENZOQUINONE PRODUCED A DEPOLARIZATION OF THE POSTSYNAPTIC MEMBRANE OF THE GIANT NEURONS IN THE 6TH ABDOMINAL GANGLION OF THE COCKROACH. THE FREQUENCY & AMPLITUDE OF UNITARY POSTSYNAPTIC POTENTIALS ALSO INCREASED. THESE EFFECTS MAY BE DUE TO INHIBITION OF ACTIVE CATION TRANSPORT. [CHAMBERS PL, ROWAN MJ; ARCH TOXICOL SUPPL 5: 107-11 (1982)] **PEER REVIEWED**

NTOX - Exptl exposure of rabbit eyes to high concn of benzoquinone vapor or direct contact with powder or concn soln has caused severe reactions with conjunctivitis, corneal edema, & necrosis. Immediately after exposure to high concn of ... vapors, a superficial brownish discoloration has been observed in exposed surfaces of ... eye, but chronic exposure of rabbits to low concn of ... vapor which were not acutely injurious has failed to induce corneal or conjunctival

pigmentation or opacities like those seen in workmen. [GRANT. TOX OF THE EYE 1986 , p. 499] **PEER REVIEWED**

NTOX - /In/ experiments with excised bovine corneas ... benzoquinone caused a loss of intercellular cohesion of the corneal epithelium upon incubation for several hours. ... Tests on rabbit lens surviving in culture in vitro have shown hydroquinone to have very little effect on cation transport or glycolysis of the lens, but showed benzoquinone to be inhibitory to both activities, despite potent antagonism to the action of benzoquinone by ascorbic acid in the lens. [GRANT. TOX OF THE EYE 1986 , p. 499] **PEER REVIEWED**

NTOX - PRETREATMENT OF FICOLL-PURIFIED RAT SPLEEN LYMPHOCYTES WITH 1,4-BENZOQUINONE ENHANCED IN VITRO PHYTOHEMAGGLUTININ (PHA)-STIMULATED MITOGENESIS AT LOWER CONCN, BUT INHIBITED LECTIN-STIMULATED BLAST FORMATION AT HIGHER CONCN. [PFEIFER RW, IRONS RD; EXP MOL PATHOL 35 (2): 189-98 (1981)] **PEER REVIEWED**

NTOX - p-Quinone was tested for mutagenicity in the Salmonella/microsome preincubation assay using the standard protocol approved by the National Toxicology Program. p-Quinone was tested at doses of 0.01, 0.03, 0.10, 0.30, 0.33, 1.0, 3.3, 10, 50, and 66 ug/plate in as many as 5 Salmonella typhimurium strains (TA1535, TA1537, TA97, TA98, and TA100) in the presence and absence of rat or hamster liver S-9. p-Quinone was negative in these tests and the highest ineffective dose tested in any S typhimurium strain was 66 ug/plate. [Mortelmans K et al; Environ Mutagen 8:1-119 (1986)] **QC REVIEWED**

HTXV - NO DATA

NTXV - NO DATA

ETXV - NO DATA

NTP - NO DATA

IARC - No data are available in humans. Inadequate evidence of carcinogenicity in animals. OVERALL EVALUATION: Group 3: The agent is not classifiable as to its carcinogenicity to humans. [IARC MONOGRAPHS. 1972-PRESENT S7 71 (1987)] **PEER REVIEWED**

TCAT - 1,4-Benzoquinone was examined for mutagenic activity in Salmonella typhimurium tester strains TA1535, TA98, TA1537, TA100 in the presence and absence of metabolic activation provided by Aroclor-induced rat liver S9 fraction. The test article was not mutagenic at concentrations ranging from 0.1 to 32 ug/plate in the absence of activation, or from 0.1 to 100 ug/plate in the presence of activation. Cytotoxicity data was not reported. [Goodyear Tire and Rubber Co.; Laboratory Report No 80-6-10 Mutagenicity Evaluation of Benzoquinone, Salmonella typhimurium/Microsome Bioassay, EPA Document No. 878210381, Fiche No. OTS0205941] **UNREVIEWED**

TCAT - Benzoquinone was examined for DNA modifying activity in Escherichia coli strains W3110 polA+ and P3478 polA- (DNA repair deficiency assay ). The test article was administered to cells by the preincubation method at concentrations of 0.01, 0.032, 0.04, 0.05 and 0.1 ug/plate in the absence of metabolic activation. The test article induced differential toxicity, as indicated by a decrease in the survival index (percent pol A- survivors divided by the percent pol A+ survivors) from 1.02 at 0.01 ug/plate to 0.07 at 0.05 ug/plate. Extreme toxicity was observed at concentrations >= 0.1 ug/ml in both E. coli strains. [Goodyear Research Division; DNA Damage by Benzoquinone (Sublimed) Sample No 8349-34 in the E. Coli Pol A1- Assay (1980), EPA Document No. 878210380, Fiche No. OTS0205941] **UNREVIEWED**

POPL - Persons with a history of congenital or acquired eye defects would be expected to be at increased risk from exposure. Persons with poor visual acuity from high degrees of astigmatism, keratoconus, or existing corneal injury should be /protected/ from repeated, uncontrolled exposure to quinone vapor. [NIOSH OSHA. OCCUPAT HEALTH GUIDE CHEM HAZARDS. 1981 , p. 1] **PEER REVIEWED**

POPL - Workers who have ... /injuries or diseases of the/ skin must be protected from work /involving 1,4-benzoquinone/. [ITI. TOX & HAZARD INDUS CHEM SAFETY MANUAL 1982 , p. 67] **PEER REVIEWED**

ADE - QUINONE IS READILY ABSORBED FROM GASTROENTERIC TRACT & SC TISSUES. IT

IS PARTIALLY EXCRETED UNCHANGED; BUT BULK IS ELIMINATED IN CONJUGATION WITH HEXURONIC, SULFURIC, & OTHER ACIDS. [PATTY. INDUS HYG & TOX 3RD ED VOL2A,2B,2C 1981-82 , p. 2593] **PEER REVIEWED**

METB - [IYANAGI T, YAMAZAKI I; BIOCHIM BIOPHYS ACTA 172: 370 (1969); KOLI AK ET AL; J BIOL CHEM 244: 621 (1969)] IN PIG PARA-QUINONE IS METABOLIZED TO P-BENZOSEMIQUINONE & QUINOL. /FROM TABLE/ [GOODWIN. HDBK INTERMED METAB AROMAT COMPD 1976 Q-5] **PEER REVIEWED**

BHL - NO DATA

ACTN - THE INFLUENCE OF P-BENZOQUINONE ON POTASSIUM UPTAKE BY EXCISED SUGAR BEET & WHEAT ROOTS WAS STUDIED. WHEN P-BENZOQUINONE WAS ADDED TO NUTRIENT SOLUTION, IT ENHANCED ABSORPTION RATES OF BOTH SPECIES AT VERY LOW CONCN WHILE INHIBITION OCCURRED FOR HIGHER CONCN. [LUCCI GC, LANDI S; AGROCHIMICA 25 (1): 20-8 (1981)] **PEER REVIEWED**

INTC - NO DATA

BION - NO DATA

THER - NO DATA

MINF - NO DATA

WARN - NO DATA

IDIO - NO DATA

TOLR - NO DATA

MXDD - NO DATA

ENVS - 1,4-Benzoquinone may be released to the environment in effluents during its commercial production and use and in wastewaters from the coal industry. If released to the soil it is susceptible to leaching (estimated Koc of 30) and may be susceptible to volatilization and photodegradation on soil surfaces. A single degradation study found benzoquinone to be rapidly degraded in a chernozem soil to stable metabolites. Sufficient data are not available to predict the significance of biodegradation in either soil or water. If released to the aquatic environment, it may be degraded by photolysis as it absorbs UV radiation. In water, benzoquinone is not expected to volatilize, adsorb to particulate matter or sediment or bioaccumulate in aquatic organisms. If released to the atmosphere in vapor-phase, it will react rapidly with both hydroxyl radicals and ozone (combined estimated half-life of 33.6 minutes) and may be susceptible to direct photolysis. Particulate associated benzoquinone released to the atmosphere may be susceptible to physical removal via dry deposition or wash-out. The ambient atmospheric concentration of benzoquinone has been reported to be less than 15 to 80 ng/cu m and benzoquinone has been detected in tobacco smoke. Inhalation appears to be the most significant route of human exposure. (SRC) [CITATION ] **PEER REVIEWED**

NATS - 1,4-Benzoquinone occurs naturally in a variety of arthropods(1). Many insects synthesize simple benzoquinones(2). [(1) IARC; Some Fumigants, the Herbicides 2,4-D and 2,4,5-T, Chlorinated Dibenzodioxins and Miscellaneous Industrial Chemicals 15: 255 (1977) (2) Thirtle JR; Kirk-Othmer Encycl Chem Tech 2nd ed John Wiley & Sons 16: 900-1 (1968)] **PEER REVIEWED**

ARTS - 1,4-Benzoquinone may be released to the environment in wastewater effluents or solid wastes generated from its commercial production(SRC). It may also be released in wastewater effluents or solid wastes produced as a result of its major commercial use as a chemical intermediate in the manufacture of hydroquinone(SRC,1). Releases may also occur from its commercial uses as a photographic chemical and tanning agent and from its use as a chemical intermediate to manufacture a variety of small volume chemicals(SRC,1). Benzoquinone can be released in wastewaters from the coal industry(2). It has been found in tobacco smoke(3). [(1) IARC; Some Fumigants, the Herbicides 2,4-D and 2,4,5-T, Chlorinated Dibenzodioxins and Miscellaneous Industrial Chemicals 15: 255 (1977) (2) Thielemann H; Z Wasser Abwasser Forsch 7: 91-3 (3) Graedel T; Chemical Compounds in the Atmosphere NY Academic Press (1978)] **PEER REVIEWED**

FATE - TERRESTRIAL FATE: 1,4-Benzoquinone was degraded very fast in a chernozem (CEC>20; BS>50) soil (persistence time not reported) leaving soil stable metabolite residues(1); the fate processes by which the

benzoquinone was degraded in this chernozem soil were not reported(SRC). Based on its log Kow value, benzoquinone is expected to have high mobility in soil predicting that leaching into groundwater is possible(SRC). Benzoquinone on soil surfaces may be susceptible to volatilization and photodegradation(SRC). Sufficient data are not available to predict the significance of biodegradation(SRC). [(1) Medvedev VA, Davydov VD; Pochvovedenie 1: 133-7 (1974)] **PEER REVIEWED**

FATE - AQUATIC FATE: Benzoquinone released to the aquatic environment is not expected to significantly volatillize adsorb to soils or sediments, or bioaccumulate in aquatic organisms. Since it absorbs UV radiation in environmentally significant wavelengths, direct photolysis is possible. Sufficient data are not available to predict the significance of biodegradation. (SRC) [CITATION ] **PEER REVIEWED**

FATE - ATMOSPHERIC FATE: Benzoquinone released to the atmosphere in vapor phase will react rapidly with both hydroxyl radicals and ozone with a combined estimated half-life of 33.6 minutes. Since it absorbs UV radiation in environmentally significant wavelengths, direct photolysis is also possible. Physical removal of benzoquinone associated with particulate matter from the atmosphere via dry deposit or wash-out may occur. (SRC) [CITATION ] **PEER REVIEWED**

BIOD - Fourteen strains of phenol-utilizing bacteria isolated from soil do not visibly grow when using 1,4-benzoquinone as a carbon source in an aqueous mineral salts media over 5 days of incubation(1). [(1) Kramer N, Doetsch RN; Arch Biochem Biophys 26: 401-5 (1950)] **PEER REVIEWED**

ABIO - The estimated half-life for the vapor-phase reaction of 1,4-benzoquinone with photochemically produced hydroxyl radicals in the atmosphere is 111.1 minutes; the estimated half-life for the vapor-phase reaction with ozone in the atmosphere is 48.1 minutes; the combined atmospheric half-life due to reaction with both hydroxyl radicals and ozone is 33.6 minutes(1). Although benzoquinone absorbs UV radiation between 300 nm to well over 400 nm(3,2), photolysis rate constants are not available for environmental parameters. Photolysis of 1,4-benzoquinone in aqueous solution using natural sunlight and artificial light in excess of 290 nm wavelength has yielded unidentifiable polar products(4). [(1) GEMS; Graphical Exposure Modeling System. Fate of atmospheric pollutants (FAP) data base. Office of Toxic Substances. USEPA (1985) (2) Sadtler; UV 248 (3) Thirtle JR; Kirk-Othmer Encycl Chem Technol 2nd ed John Wiley and Sons NY 16: 900-1 (1968) (4) Ware GW et al; Arch Environ Contam Toxicol 9: 135-46 (1980)] **PEER REVIEWED**

BIOC - Based on a log Kow value of 0.20(1), the bioconcentration factor (BCF) for benzoquinone can be estimated to be about 0.84 (log BCF= -0.078) by use of a recommended regression equation(2,SRC). [(1) Hansch C, Leo AJ; Medchem Project Issue no. 26 Claremont CA Pomona College (1985) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. McGraw-Hill NY (1982)] **PEER REVIEWED**

KOC - Based on a log Kow value of 0.20(1), the Koc value for benzoquinone can be estimated to be about 30, indicating high mobility in soil(2,SRC). [(1) Hansch C, Leo AJ; Medchem Project Issue no. 26 Claremont CA Pomona College (1985) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. McGraw-Hill NY (1982)] **PEER REVIEWED**

VWS - The Henry's Law constant for benzoquinone at 25 deg C is estimated to be 4X10-7 atm-cu m/mol(1,SRC). The Henry's Law constant for benzoquinone has been estimated to be 1.8X10-7 atm-cu m/mol from a calculated water solubility (based on log Kow= 0.20) and measured (at 25 deg C) vapor pressure(2). Volatilization can be considered unimportant as an aqueous-air transfer mechanism based on the low Henry's Law constant(2). Benzoquinone sublimes(3) and has a vapor pressure of 0.09 mm Hg at 20 deg C(4) suggesting that volatilization of solid particles from soil surfaces may be a significant transfer mechanism(SRC). [(1) Hine J, Mookerjee PK; J Org Chem 40: 292-8 (1975)

(2) GEMS; Graphical Exposure Modeling System. Chemical Estimation (CHEMEST) data base. Office of Toxic Substances. USEPA (1986) (3) IARC; Some Fumigants, the Herbicides 2,4-D and 2,4,5-T, Chlorinated Dibenzodioxins and Miscellaneous Industrial Chemicals 15: 255 (1977) (4) Verschueren K; Handbook of environmental data on organic chemicals. 2nd ed Von Nostrand Reinhold NY (1983) ] **PEER REVIEWED**

WATC - SURFACE WATER: /1,4-Benzoquinone/ ... has been found as a pollutant in filtered surface ... water at a water treatment plant. [IARC MONOGRAPHS. 1972-PRESENT V15 257 (1977)] **PEER REVIEWED**

WATC - GROUNDWATER: /1,4-Benzoquinone/ ... has been found as a pollutant in filtered ... ground water at a water treatment plant. [IARC MONOGRAPHS. 1972-PRESENT V15 257 (1977)] **PEER REVIEWED**

EFFL - NO DATA

SEDS - NO DATA

ATMC - The ambient atmospheric concentration of 1,4-benzoquinone has been reported to be less than 15 to 80 ng/cu m(1). 1,4-Benzoquinone has been detected in tobacco smoke(1). [(1) Graedel TE; Chemical Compounds in the Atmosphere New York, NY Academic Press (1978)] **PEER REVIEWED**

FOOD - NO DATA

PLNT - NO DATA

FISH - NO DATA

ANML - NO DATA

MILK - NO DATA

OEVC - NO DATA

RTEX - Inhalation of contaminated air, especially near areas of use and production, may provide significant exposure. Inhalation exposure is possible as a result of tobacco smoking. (SRC) [CITATION ] **PEER REVIEWED**

RTEX - Quinone can affect the body if it ... comes in contact with the eyes or skin. It can also affect the body if it is swallowed. [NIOSH OSHA. OCCUPAT HEALTH GUIDE CHEM HAZARDS. 1981 , p. 1] **PEER REVIEWED**

=VDI - NO DATA

PBEX - ... WORKERS ENGAGED IN MFR OF HYDROQUINONE ... /ARE EXPOSED TO/ COLORLESS HYDROQUINONE DUST ... [CASARETT AND DOULL'S TOXICOLOGY 3RD ED 1986 , p. 483] **PEER REVIEWED**

PBEX - NIOSH (NOHS Survey 1972-1974) has statistically estimated that 3747 workers are exposed to 1,4-benzoquinone in the USA(1). [(1) NIOSH; National Occupational Survey Hazard. NOHS (1974)] **PEER REVIEWED**

PBEX - The following list includes some common operations in which exposure to quinone may occur ... : Use as oxidizing agent ... in photography ... in agriculture production of insecticides & fungicides; in pharmaceutical industry for production of cortisone & addition cmpd with barbiturates; use in polymer & resins industry .. use as toner & intensifier in photographic industry; as a tanning agent for leather industry; use in mfr of quinhydrone electrodes for use for pH determinations. [NIOSH OSHA. OCCUPAT HEALTH GUIDE CHEM HAZARDS. 1981 , p. 3] **PEER REVIEWED**

BODY - NO DATA

IDLH - 300 mg/cu m [NIOSH. NIOSH POCKET GUIDE CHEM HAZ 1990 , p. 192] **QC REVIEWED**

ADI - NO DATA

ATOL - NO DATA

OSHA - Meets criteria for OSHA medical records rule. [29 CFR 1910.20 (7/1/88)] **PEER REVIEWED**

OSHA - 8 hr Time-Weighted avg: 0.1 ppm (0.4 mg/cu m) [29 CFR 1910.1000 (7/1/88)] **PEER REVIEWED**

NREC - NO DATA

TLV - Time Weighted Avg (TWA) 0.1 ppm, 0.44 mg/cu m (1987) [ACGIH. TLV'S & BIOLOGICAL EXP INDICIES 1991-92 , p. 32] **QC REVIEWED**

TLV - Excursion Limit Recommendation: Excursions in worker exposure levels may exceed three times the TLV-TWA for no more than a total of 30 min during a work day and under no circumstances should they exceed five times the TLV-TWA, provided that the TLV-TWA is not exceeded. [ACGIH. TLV'S & BIOLOGICAL EXP INDICIES 1991-92 , p. 5] **QC REVIEWED**

OOPL - OSHA's health standards for exposure to air contaminants require that employees exposure to para-quinone does not exceed 8-hr time-weighted avg of 0.1 ppm (0.4 mg/cu m). ... The corresponding standard in the Federal Republic of Germany & in Australia is also 0.4 mg/cu m, & the acceptable ceiling concn in USSR is 0.05 mg/cu m. [IARC MONOGRAPHS. 1972-PRESENT V15 257 (1977)] **PEER REVIEWED**
WSTD - NO DATA
ASTD - This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to use the best demonstrated system of continuous emission reduction for equipment leaks of VOC, considering costs, non air quality health and environmental impact and energy requirements. 1,4-Benzoquinone is produced, as an intermediate or final product, by process units covered under this subpart. [40 CFR 60.489 (7/1/87)] **PEER REVIEWED**
SSTD - NO DATA
CERC - Persons in charge of vessels or facilities are required to notify the National Response Center (NRC) immediately, when there is a release of this designated hazardous substance, in an amount equal to or greater than its reportable quantity of 10 lb or 4.45 kg. The toll free telephone number of the NRC is (800) 424-8802; In the Washington metropolitan area (202) 426-2675. The rule for determining when notification is required is stated in 40 CFR 302.6 (section IV. D.3.b). [40 CFR 302.4 (7/1/88).] **PEER REVIEWED**
TSCA - Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. 1,4-Benzoquinone is included on this list. [40 CFR 716.120 (7/1/88)] **PEER REVIEWED**
TSCA - Section 8(a) of TSCA requires manufacturers of this chemical substance to report preliminary assessment information concerned with production, use, and exposure to EPA. [40 CFR 712.30 (7/1/88)] **PEER REVIEWED**
RCRA - As stipulated in 40 CFR 261.33, when quinones, as a commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or a manufacturing chemical intermediate, becomes a waste, it must be managed according to Federal and/or State hazardous waste regulations. Also defined as a hazardous waste is any residue, contaminated soil, water, or other debris resulting from the cleanup of a spill, into water or on dry land, of this waste. Generators of small quantities of this waste may qualify for partial exclusion from hazardous waste regulations (40 CFR 261.5). [40 CFR 261.33 (7/1/88)] **PEER REVIEWED**
FIFR - NO DATA
FDA - NO DATA

1 - IRIS
NAME - Quinone
RN - 106-51-4
---
CAA - NO DATA
---
WQCHU- NO DATA
---
WQCAQ- NO DATA
---
MCLG - NO DATA
---
MCL - NO DATA
---
SMCL - NO DATA

**Table C-1**

| Numeric Toxicity Data for TRI Chemicals | | REFERENCE DOSES VALUES mg/kg-d | | | | FRESH WATER CHRONIC CRITERIA | | CANCER POTENCY VALUES Risk/mg/kg-d[g] | | | | WEIGHT OF EVIDENCE | | NON-CONVENTIONAL DATA SOURCES AVAILABLE DATA Risk/mg/kg-d | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CAS | CHEMICAL | INHALATION | | ORAL | | (ug/L) | | INHALATION | | ORAL | | INHAL | ORAL | RQ | CA | OPP/PF | |
| 75070 | ACETALDEHYDE | 2 6E-03 | | | | | | 7.70E-03 | | | | B2 | | | | | |
| 60355 | ACETAMIDE | | | | | | | | | | | | o | | 0.07 | 148 | B2 |
| 67641 | ACETONE | | | 1.0E-01 | | | | | | | | | | | | | |
| 75058 | ACETONITRILE | 1.0E-02 | b | 6 0E-03 | | | | | | | | | | | | | |
| 53963 | ACETYLAMINOFLUORENE,2 | | | | | | | | | | | | B2 | | | | |
| 107028 | ACROLEIN | 5.7E-06 | | 0.02 | b | 21 | e | | | | | | | | | | |
| 79061 | ACRYLAMIDE | ND | | 2 0E-04 | | | | 4 5 | | 4.5 | | B2 | B2 | | | | |
| 79107 | ACRYLIC ACID | 8 6E-05 | | 8.0E-02 | | | | | | | | | | | | | |
| 107131 | ACRYLONITRILE | | | | | 2600 | | 2.40E-01 | | 5.40E-01 | | B1 | B1 | | | | |
| 309002 | ALDRIN | ND | | 3.0E-05 | | | | 1.70E+01 | | 1.70E+01 | | B2 | B2 | | | | |
| 107051 | ALLYL CHLORIDE | 2.9E-04 | b | 0.05 | b | 0.001 | b | | | | | | | | | | |
| 7429905 | ALUMINUM | | | | | | | | | | | | | x | | | |
| 117793 | AMINOANTHRAQUINONE,2 | | | | | | | | | | | | | | 0 033 | | |
| 60093 | AMINOAZOBENZENE, 4 | | | | | | | | | | | | | | | | |
| 92671 | AMINODIPHENYL,4 | | | | | | | | | | | | | | 0 26 | | |
| 82280 | 1-AMINO 2-METHYL-ANTHRAQUINONE | | | | | | | | | | | | | | 0 15 | | |
| 7664417 | AMMONIA | 2 9E-02 | | 9.7E-01 | s | | | | | | | | | | | | |
| 6484522 | AMMONIUM NITRATE | | | | | | | | | | | | | | | | |
| 7783202 | AMMONIUM SULFATE | | | | | | | | | | | | | | | | |
| 62533 | ANILINE | 2 9E-04 | | ND | | | | | | 5.70E-03 | | B2 | B2 | | | | |
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| 134292 | ANISIDINE HYDROCHLORIDE,O | | | | | | | | | | | | | | 0 11 | | |
| 120127 | ANTHRACENE | ND | | 3 0E-01 | | | | | | | | | | | | | |
| 7440360 | ANTIMONY | | | 4.0E-04 | | 1600 | | | | | | | | | | | |
| 20008 | ANTIMONY COMPOUNDS* | ND | | 4.0E-04 | | | | | | | | | | | | | |
| 7440382 | ARSENIC | | | 3.0E-04 | | 190 | | 1.50E+01 | | | | A | | | | | |
| 20019 | ARSENIC COMPOUNDS* | | | 3.0E-04 | | | | 1.50E+01 | | | | A | | | | | |
| 1332214 | ASBESTOS | | | | | | | 2.30E-02 | m | | | A | | | | | |
| 492808 | AURAMINE | | | | | | | | | | | | | x | 0.03 | 0.48 | B2 |
| 7440393 | BARIUM | 1.0E-04 | b | 7.0E-02 | | | | | | | | | | | | | |
| 20020 | BARIUM COMPOUNDS* | 1.0E-04 | b | 7.0E-02 | | | | | | | | | | | | | |
| 98873 | BENZAL CHLORIDE | | | | | | | | | | | | | x | | | |
| 55210 | BENZAMIDE | | | | | | | | | | | | | | | | |
| 71432 | BENZENE | | | | | | | 2.90E-02 | | 2.90E-02 | | A | A | | | | |
| 92875 | BENZIDINE | | | 3.0E-03 | | | | 2.30E+02 | | 2 30E+02 | | A | A | | | | |
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| 98077 | BENZOTRICHLORIDE | | | | | | | | | 1.30E+01 | | | B2 | | | | |
| 98884 | BENZOYL CHLORIDE | | | | | | | | | 0 66 | | | B2 | | | | |

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| 100447 | BENZYL CHLORIDE | | | | | | | | | 1.70E-01 | | | | B2 | |
| 7440417 | BERYLLIUM | | | 5.0E-03 | | 5.3 | | 8.40E+00 | | 4.30E+00 | | B2 | | B2 | |
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| 108601 | BIS(2CHLORO1METHETHYL)ETHER | | | | | | | 7.00E-02 | b | 7.00E-02 | b | C | b | C | b |
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| 542881 | BIS(CHLOROMETHYL)ETHER | | | | | | | 2.20E+02 | | 2.20E+02 | | A | | A | |
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| 75650 | BUTYL ALCOHOL, TERT | | | 1 | p | | | | | | | | | | |
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| 58899 | LINDANE (HEXACHLOROCYCLOHEXANE, GA | | | 3 0E-04 | | 0.06 | e | | | | | | | | | | | | |
| 108316 | MALEIC ANHYDRIDE | ND | | 1.0E-01 | | | | | | | | | | | | | | | |
| 12427382 | MANEB | ND | | 5.0E-02 | b | | | | | | | | | | | | | | |
| 7439965 | MANGANESE | 1.1E-04 | | 1.0E-01 | | | | | | | | D | | | | | | | |
| 20122 | MANGANESE COMPOUNDS* | 1.1E-04 | | 1.0E-01 | | | | | | | | | | | | | | | |
| 7439976 | MERCURY | 3 0E-04 | b | 3.0E-04 | b | 0.012 | e | | | | | | | | | | | | |
| 20133 | MERCURY COMPOUNDS* | 3 0E-04 | b | 3.0E-04 | b | | | | | | | | | | | | | | |
| 67561 | METHANOL | ND | | 5.0E-01 | | | | | | | | | | | | | | | |
| 72435 | METHOXYCHLOR | ND | | 5.0E-03 | | 0.03 | e | | | | | | | | | | | | |
| 109864 | METHOXYETHANOL, 2 | 5.7E-03 | | | | | | | | | | | | | | | | | |
| 96333 | METHYL ACRYLATE | ND | | 3.0E-02 | b | | | | | | | | | | | | | | |
| 78933 | METHYL ETHYL KETONE | 9 0E-02 | b | 5.0E-02 | b | | | | | | | | | | | | | | |
| 60344 | METHYL HYDRAZINE | | | | | | | | | 1.10E+00 | b | | | NA | | | | | |
| 74884 | METHYL IODIDE | | | | | | | | | | | | | C | u | | | | |
| 108101 | METHYL ISOBUTYL KETONE | 2 0E-02 | b | | | | | | | | | | | | | | | | |
| 624839 | METHYL ISOCYANATE | | | | | | | | | | | | | | | x | | | |
| 80626 | METHYL METHACRYLATE | | | | | | | | | | | | | | | x | | | |
| 1634044 | METHYL TERTBUTYL ETHER | | | 0 0052 | l | | | | | | | | | | | | | | |
| 74953 | METHYLENE BROMIDE (DIBROMOMETHANE) | ND | | 0.01 | v | | | | | | | | | | | | | | |
| 101144 | METHYLENEBIS(2CHLORO ANILINE) | | | | | | | 1.30E-01 | b | 1.30E-01 | b | B2 | b | B2 | b | | | | |
| 101611 | METHYLENEBIS(N,N,DIMETHYL)BENZENAMINE | | | | | | | | | 4 60E-02 | | | | B2 | | | | | |
| 101688 | METHYLENEBIS(PHENYLISOCYANATE) | | | | | | | | | | | | | | | | | | |
| 101779 | METHYLENEDIANILINE,4,4 | | | | | | | | | | | | | | | | 1.6 | | |
| 90948 | MICHLERS KETONE | | | | | | | | | | | | | | | | 0 86 | | |
| 1313275 | MOLYBDENUM TRIOXIDE | | | | | | | | | | | | | | | | | | |
| 505602 | MUSTARD GAS | | | | | | | | w | | w | | | | | x | | | |
| 91203 | NAPHTHALENE | ND | | 4 0E-03 | b | 620 | e | | | | | | | | | | | | |
| 134327 | NAPHTHYLAMINE, ALPHA | | | | | | | | | N/A | | | | C | | | | | |
| 91598 | NAPHTHYLAMINE, BETA | | | | | | | | | 4.77 | | | | A | | | | | |
| 7440020 | NICKEL | | | 2.0E-02 | | 160 | e | 1.70E+00 | b | | | A | b | | | | | | |
| 20144 | NICKEL COMPOUNDS* | ND | | 2.0E-02 | | | | 1.70E+00 | b | | | A | b | | | | | | |
| 7697372 | NITRIC ACID | | | | | | | | | | | | | | | x | | | |
| 139139 | NITRILOTRIACETIC ACID | | | | | | | | | | | | | | | | 0.005 | | |
| 98953 | NITROBENZENE | 2 0E-03 | b | 5 0E-04 | | | | | | | | | | | | | | | |
| 92933 | NITROBIPHENYL,4 | | | | | | | | | | | | | | | | | | |
| 1836755 | NITROFEN | | | | | | | | | | | | | | | | 0.082 | | |
| 51752 | NITROGEN MUSTARD | | | | | | | | x | | x | | | | | x | | | |
| 55630 | NITROGLYCERIN | | | | | | | | | | | | | | | | | | |
| 99592 | NITROOANISIDINE, 5 | | | | | | | | y | | y | | | | | | 0.049 | | |
| 88755 | NITROPHENOL,2 | | | | | 150 | e | | | | | | | | | | | | |

Refer to end of table for citations

| | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 100027 | NITROPHENOL,4 | | | | | 150 | e | | | | | | | | | | | | | | | | |
| 79469 | NITROPROPANE, 2 | 5 7E-03 | | ND | | | | 9.40E+00 | b | 9 50E+00 | b | B2 | b | B2 | b | | | | | | | | |
| 55185 | NITROSODIETHYLAMINE,N | | | | | | | 1.50E+02 | | 1 50E+02 | | B2 | | B2 | | | | | | | | | |
| 62759 | NITROSODIMETHYLAMINE,N | | | | | | | 5 10E+01 | | 5 10E+01 | | B2 | | B2 | | | | | | | | | |
| 924163 | NITROSODI-n-BUTYLAMINE,N | | | | | | | 5 40E+00 | | 5 40E+00 | | B2 | | B2 | | | | | | | | | |
| 621647 | NITROSODI-n-PROPYLAMINE,N | | | | | | | | | 7 00E+00 | | | | B2 | | | | | | | | | |
| 156105 | NITROSODIPHENYLAMINE, P | | | | | | | | | | | | | | | | 0 022 | | | | | | |
| 86306 | NITROSODIPHENYLAMINE,N | | | | | | | | | 4 90E-03 | | | | B2 | | | | | | | | | |
| 4549400 | NITROSOMETHYLVINYLAMINE,N | | | | | | | | | | | | | | | x | | | | | | | |
| 59892 | NITROSOMORPHOLINE,N | | | | | | | | | | | | | | | | 6 7 | | | | | | |
| 759739 | NITROSO-N-ETHYLUREA,N | | | | | | | | | | | | | | | x | | 137 | B2 | | | | |
| 684935 | NITROSO-N-METHYLUREA,N | | | | | | | | | | | | | | | x | | 2100 | B2 | | | | |
| 16543558 | NITROSONORNICOTINE,N | | | | | | | | | | | | | | | | 1.4 | | | | | | |
| 100754 | NITROSOPIPERIDINE,N | | | | | | | | | | | | | | | x | 9 4 | 37 5 | B2 | | | | |
| 2234131 | OCTACHLORONAPHTAHLENE | | | | | | | | | | | | | | | | | | | | | | |
| 20816120 | OSMIUM TETROXIDE | | | | | | | | z | | z | | | | | x | | | | | | | |
| 56382 | PARATHION | ND | | 6.0E-03 | b | 0.013 | d | | | | | C | | C | | | | | | | | | |
| 87865 | PENTACHLOROPHENOL | ND | | 3.0E-02 | | 13 | | | | 1.20E-01 | | | | B2 | | | | | | | | | |
| 79210 | PERACETIC ACID | | | | | | | | | | | | | | | x | | | | | | | |
| 108952 | PHENOL | ND | | 6.0E-01 | | 2560 | | | | | | | | | | | | | | | | | |
| 106503 | PHENYLENEDIAMINE,P | | | 0.19 | b | | | | | | | | | | | | | | | | | | |
| 90437 | PHENYLPHENOL, 2 | | | | | | | | | 1.90E-03 | b | C | b | C | b | | | | | | | | |
| 75445 | PHOSGENE | | | | | | | | | | | | | | | x | | | | | | | |
| 7664382 | PHOSPHORIC ACID | | | | | | | | | | | | | | | x | | | | | | | |
| 7723140 | PHOSPHORUS (YELLOW OR WHITE) | | | 2 0E-05 | | | | | | | | | | | | | | | | | | | |
| 85449 | PHTHALIC ANHYDRIDE | ND | | 2 0E+00 | | | | | | | | | | | | | | | | | | | |
| 88891 | PICRIC ACID (2,4,6TRINITROPHENOL) | | | | | | | | | | | | | | | | | | | | | | |
| 1336363 | POLYCHLORINATED BIPHENYLS | | | | | | | | | 7 70E+00 | | | | B2 | | | | | | | | | |
| 1120714 | PROPANE SULTONE | | | | | | | | | 10 | | | | B2 | | | | | | | | | |
| 57578 | PROPIOLACTONE,BETA | | | | | | | | | | | | | | | x | 14 | | | | | | |
| 123386 | PROPIONALDEHYDE | | | | | | | | | | | | | | | | | | | | | | |
| 114261 | PROPOXUR (BAYGON) | | | 4.00E-03 | | | | | | | | | | | | | | | | | | | |
| 75569 | PROPYLENE OXIDE | 8 6E-03 | | ND | | | | 0.013 | | 2.40E-01 | | | | B2 | | | | | | | | | |
| 115071 | PROPYLENE (PROPENE) | | | | | | | | | | | | | | | | | | | | | | |
| 75558 | PROPYLENEIMINE | | | | | | | | | | | | | | | x | | 259 | B2 | | | | |
| 110861 | PYRIDINE | ND | | 1.0E-03 | | | | | | | | | | | | | | | | | | | |
| 91225 | QUINOLINE | | | | | | | | | 1.20E+01 | b | C | b | C | b | | | | | | | | |
| 82688 | QUINTOZENE (PENTACHLORONITROBENZEN | | | 3.0E-03 | | | | | | | | | | | | | | | | | | | |
| 81072 | SACCHARIN (MANUFACTURING) | | | | | | | | | | | | | | | x | | 0.007 | C | | | | |
| 94597 | SAFROLE | | | | | | | | | | | | | | | x | 0.22 | 0.18 | B2 | | | | |
| 7782492 | SELENIUM | | | 5.0E-03 | | 35 | e | | | | | | | | | | | | | | | | |
| 7440224 | SILVER | ND | | 3.0E-03 | b | 0.12 | e | | | | | | | | | | | | | | | | |
| 20177 | SILVER COMPOUNDS* | ND | | 3 0E-03 | b | | | | | | | | | | | | | | | | | | |
| 100425 | STYRENE | ND | | 2 0E-01 | | | | 2 00E-03 | b | 3 00E-02 | b | B2 | b | B2 | b | | | | | | | | |
| 96093 | STYRENE OXIDE | | | | | | | | | | | | | | | | 0.16 | | | | | | |
| 7664939 | SULFURIC ACID | ND | | ND | | | | | | | | | | | | | | | | | | | |
| 79345 | TETRACHLOROETHANE, 1,1,2,2 | | | 3 0E-02 | b | 2400 | e | 2 00E-01 | | 2.00E-01 | | C | | C | | | | | | | | | |
| 127184 | TETRACHLOROETHYLENE (PERCHLORETHYL | ND | | 1.0E-02 | | 840 | | | | 5.10E-02 | b | B2 | g | B2 | b | | | | | | | | |

Refer to end of table for citations

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 96111[illegible] | [illegible]TRACHLORVINPHOS | ND | | 3 0E-[illegible] | | | | | | | | | | | | | | | |
| 74402[illegible] | [illegible]ALLIUM | | | 7 0E[illegible] | | 40 | e | | | | | | | | | | | | |
| 6255[illegible] | [illegible]OACETAMIDE | | | | | | | | | | | | | | | x | | 24 8 | B2 |
| 139651 | THIODIANILINE,4,4 | | | | | | | | | | | | | | | | [illegible] | | |
| 62566 | THIOUREA | | | | | | | | | | | | | | | x | 0 072 | 1 05 | |
| 1314201 | THORIUM DIOXIDE | | | | | | | | | | | | | | | | | | |
| 7550450 | TITANIUM TETRACHLORIDE | | | | | | | | | | | | | | | x | | | |
| 108883 | TOLUENE | 5 7E-01 | b | 2.0E-01 | | | | | | | | | | | | | | | |
| 584849 | TOLUENE2,4DIISOCYANATE | | | | | | | | | | | | | | | x | 0 039 | | |
| 91087 | TOLUENE2,6DIISOCYANATE | | | | | | | | | | | | | | | | 0 039 | | |
| 95534 | TOLUIDINE, O | | | | | | | | | 2.40E-01 | b | | | B2 | b | | | | |
| 636215 | TOLUIDINE HYDROCHLORIDE | | | | | | | | | | | | | | | x | 0 13 | | |
| 8001352 | TOXAPHENE | | | | | 0.000 | e | 1.10E+00 | | 1.10E+00 | | B2 | | B2 | | | | | |
| 68768 | TRIAZIQUONE | | | | | | | | | | | | | | | | | | |
| 52686 | TRICHLORFON | | | 0.01 | # | | | | | | | | | | | | | | |
| 120821 | TRICHLOROBENZENE, 1,2,4 | | | 1 0E-02 | b | 50 | | | | | | | | | | | | | |
| 71556 | TRICHLOROETHANE, 1,1,1 | 3 0E-01 | b | 9 0E-02 | b | 31200 | e | | | | | | | | | | | | |
| 79005 | TRICHLOROETHANE, 1,1,2 | | | 4.0E-03 | | 9400 | | 0 057 | | 5.70E-02 | | | | C | | | | | |
| 79016 | TRICHLOROETHYLENE | | | 7.00E-03 | g | 21900 | | 1.70E-02 | | 1.10E-02 | | B2 | | B2 | | | | | |
| 95954 | TRICHLOROPHENOL, 2,4,5 | ND | | 1.0E-01 | | | | | | | | | | | | | | | |
| 88062 | TRICHLOROPHENOL, 2,4,6 | | | | | 970 | | 1.10E-02 | | 1.10E-02 | | B2 | | B2 | | | | | |
| 1582098 | TRIFLURALIN | ND | | 7 5E-03 | | | | | | 7.70E-03 | | | | C | | | | | |
| 95636 | TRIMETHYLBENZENE, 1,2,4 | | | | | | | | | | | | | | | | | | |
| 126727 | TRIS(2,3DIBROMOPROPYL)PHOSPHATE | | | | | | | | | 9.76 | | | | B2 | | | | | |
| 51796 | URETHANE (ETHYL CARBAMATE) | | | | | | | | | 0 64 | | | | B2 | | | | | |
| 7440622 | VANADIUM | | | 7.0E-03 | b | | | | | | | | | | | | | | |
| 108054 | VINYL ACETATE | 5 7E-02 | | 1 0E+00 | b | | | | | | | | | | | | | | |
| 593602 | VINYL BROMIDE | | | | | | | 1.10E-01 | b | | | B2 | b | B2 | b | | | | |
| 75014 | VINYL CHLORIDE | | | | | | | 0.3 | b | 1.90E+00 | b | A | b | A | b | | | | |
| 75354 | VINYLIDENE CHLORIDE (1,1 DICHLOROETHYL | | | 9 0E-03 | | | | | | 6 00E-01 | | | | C | | | | | |
| 108383 | XYLENE, M | 2 0E-01 | b | 2 0E+00 | b | | | | | | | | | | | | | | |
| 95476 | XYLENE, O | 2 0E-01 | b | 2 0E+00 | b | | | | | | | | | | | | | | |
| 106423 | XYLENE, P | 8 6E-02 | b | ND | | | | | | | | | | | | | | | |
| 1330207 | XYLENE (MIXED ISOMERS) | 8.6E-02 | d | 2.0E+00 | | | | | | | | | | | | | | | |
| 87627 | XYLIDINE,2,6 | | | | | | | | | | | | | | | | | | |
| 7440666 | ZINC | 0 7 | c | 2.0E-01 | b | 110 | e | | | | | | | | | | | | |
| 20199 | ZINC COMPOUNDS* | 0.7 | c | 2 0E-01 | b | 110 | e | | | | | | | | | | | | |
| 12122677 | ZINEB | ND | c | 5.0E-02 | | | | | | | | | | | | | | | |

KEY TO FOOTNOTES

All numbers are IRIS unless otherwise specified

* See individual element for data on compounds
NOTE: For metal compounds, the toxicity data presented in the table are those of the parent compound.

a = IRIS
b = HEAST (data used first from 1992 tables, but if references were unavailable, 1991 HEAST tables were used)

c = RSG
d = ECTOX
e = WQCS
f = CURE
g = represents an upperbound estimate of risk
h = used para-cresol form to determine value
i = value is for refinery dust
j = data available are inadequate for calculating potency factor, no quantitative inferences can be made
k = BCME data per IRIS
l = Abt figure
m = fibers/ml raised -1m
n = based on the glycool ether 2-methoxyethanol
o = OPP assigned this a class C carcinogen based on male/female rat liver tumors
p = based on n-butyl alcohol
q = RfD inhalation value is based on water not on food
r = Cancer classification of medium potency is basis for final RQ
s = calculated from HEAST data
t = OPP assigned class C/B2 carcinogen; no quantitative data
u = No adequate quantitative data so assigned to middle cancer potency group
v = based on similarity to bromoform and methyl bromide; in HEAST
w = Not found on EPA list; however, extensive RTECS citations (#79634); IARC cancer review - sufficient animal evidence, limited human evidence; quantitative data available but not in PF form
x = Extensive citations in RTECS (#31472), including numerous carcinogenicity studies; no PF available
y = Extensive citations in RTECS (#8628), NCI carcinogenicity bioassay - clear evidence; no PF available
z = RTECS (#53213) indicates reproductive hazard
# = WHO data, Note. conflicting Oral RfD = 0 125 from OPP

**Table C-2**

| Numeric Toxicity Data for TRI Chemicals | | REPORTABLE QUANTITIES (POUNDS) | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| CAS | CHEMICAL | CANCER | | CHRONIC | | ACUTE | | AQUATIC | |
| 75070 | ACETALDEHYDE | | | | | 5000 | | 1000 | |
| 60355 | ACETAMIDE | | | | | | | | |
| 67641 | ACETONE | | | | | | | 5000 | a |
| 75058 | ACETONITRILE | | | 1000 | a | 5000 | a | 5000 | |
| 53963 | ACETYLAMINOFLUORENE,2 | 1 | | | | 5000 | | | |
| 107028 | ACROLEIN | | | | | 100 | | 1 | |
| 79061 | ACRYLAMIDE | | | | | 5000 | | | |
| 79107 | ACRYLIC ACID | | | | | 5000 | a | | |
| 107131 | ACRYLONITRILE | 10 | a | 100 | | 1000 | | 100 | |
| 309002 | ALDRIN | 1 | a | | | 1000 | | 1 | a |
| 107051 | ALLYL CHLORIDE | | | | | 1000 | | 1000 | |
| 7429905 | ALUMINUM | | | 1000 | | | | | |
| 117793 | AMINOANTHRAQUINONE,2 | | | | | | | | |
| 60093 | AMINOAZOBENZENE, 4 | | | | | | | | |
| 92671 | AMINODIPHENYL,4 | | | | | | | | |
| 82280 | 1-AMINO 2-METHYL-ANTHRAQUINONE | | | | | | | | |
| 7664417 | AMMONIA | | | 1000 | | 5000 | | 10 | |
| 6484522 | AMMONIUM NITRATE | | | | | | | | |
| 7783202 | AMMONIUM SULFATE | | | | | | | | |
| 62533 | ANILINE | | | | | 1000 | | 1000 | |
| 90040 | ANISIDINE,O | | | | | | | | |
| 104949 | ANISIDINE,P | | | | | | | | |
| 134292 | ANISIDINE HYDROCHLORIDE,O | | | | | | | | |
| 120127 | ANTHRACENE | | | | | | | | |
| 7440360 | ANTIMONY | | | | | 5000 | a | | |
| 20008 | ANTIMONY COMPOUNDS* | | | | | | | | |
| 7440382 | ARSENIC | 1 | | | | | | | |
| 20019 | ARSENIC COMPOUNDS* | | | | | | | | |
| 1332214 | ASBESTOS | 1 | | 10 | | | | | |
| 492808 | AURAMINE | 100 | | | | | | | |
| 7440393 | BARIUM | | | | | 100 | e | | |
| 20020 | BARIUM COMPOUNDS* | | | | | | | | |
| 98873 | BENZAL CHLORIDE | | | | | 5000 | | | |
| 55210 | BENZAMIDE | | | | | | | | |
| 71432 | BENZENE | 10 | a | 1000 | | 5000 | | 100 | |
| 92875 | BENZIDINE | 1 | a | 100 | | 5000 | | 100 | |
| 106514 | BENZOQUINONE (QUINONE) | | | | | 5000 | | 10 | |
| 98077 | BENZOTRICHLORIDE | 10 | | | | 1000 | | | |
| 98884 | BENZOYL CHLORIDE | | | | | | | 1000 | |

Refer to of table for citations

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9436 | IZOYL PEROXIDE | | | | | | | | | | |
| 10044 | NZYL CHLORIDE | 100 | | | | 00 | | 100 | | | |
| 7440417 | BERYLLIUM | 10 | | | | | | 1000 | | | |
| 92524 | BIPHENYL (DIPHENYL) | | | | | | | | | | |
| 111444 | BIS(2CHLOROETHYL)ETHER | 10 | | | | 1000 | | 5000 | | | |
| 108601 | BIS(2CHLORO1METHETHYL)ETHER | | | 1000 | | 5000 | | | | | |
| 103231 | BIS(2ETHYLHEXYL)ADIPATE | | | | | | | | | | |
| 542881 | BIS(CHLOROMETHYL)ETHER | 1 | | | | 100 | | | | | |
| 75252 | BROMOFORM (TRIBROMOMETHANE) | | | 100 | a | 5000 | | 1000 | | | |
| 74839 | BROMOMETHANE (METHYL BROMIDE) | | | | | 1000 | a | 5000 | | | |
| 106990 | BUTADIENE, 1,3 | 1 | a | | | | | | | | |
| 141322 | BUTYL ACRYLATE | | | | | | | | | | |
| 71363 | BUTYL ALCOHOL, N (BUTANOL) | | | | | 5000 | a | | | | |
| 78922 | BUTYL ALCOHOL, SEC | | | | | | | | | | |
| 75650 | BUTYL ALCOHOL, TERT | | | | | | | | | | |
| 85687 | BUTYL BENZYL PHTHALATE | | | | | | | 100 | | | |
| 106887 | BUTYLENE OXIDE, 1,2 | | | | | | | | | | |
| 123728 | BUTYRALDEHYDE | | | | | | | | | | |
| 7440439 | CADMIUM | 10 | a | | | 5000 | | | | | |
| 20042 | CADMIUM COMPOUNDS* | | | | | | | | | | |
| 156627 | CALCIUM CYANAMIDE | | | | | | | | | | |
| 133062 | CAPTAN | | | 1000 | | 5000 | | 10 | | | |
| 63252 | CARBARYL | | | | | 5000 | | 100 | a | | |
| 75150 | CARBON DISULFIDE | | | 100 | a | 1000 | | 5000 | | | |
| 56235 | CARBON TETRACHLORIDE | 10 | a | 100 | | 5000 | | 1000 | | | |
| 463581 | CARBONYL SULFIDE | | | | | | | | | | |
| 120809 | CATECHOL (1,2 DIHYDROXYBENZENE) | | | | | | | | | | |
| 133904 | CHLORAMBEN | | | | | | | | | | |
| 57749 | CHLORDANE | 10 | | | | 1000 | | 1 | a | | |
| 7782505 | CHLORINE | | | | | 1000 | | 10 | | | |
| 10049044 | CHLORINE DIOXIDE | | | | | | | | | | |
| 79118 | CHLOROACETIC ACID | | | 100 | | 1000 | | | | | |
| 532274 | CHLOROACETOPHENONE | | | | | | | | | | |
| 108907 | CHLOROBENZENE | | | 1000 | | 5000 | | 100 | | | |
| 510156 | CHLOROBENZILATE | 10 | | | | 5000 | | | | | |
| 75003 | CHLOROETHANE (ETHYL CHLORIDE) | | | | | 5000 | | 5000 | | | |
| 67663 | CHLOROFORM | 10 | a | | | 5000 | | 1000 | | | |
| 74873 | CHLOROMETHANE | 100 | | 1000 | | 5000 | | 5000 | | | |
| 107302 | CHLOROMETHYL METHYL ETHER | 1 | | 100 | | 1000 | | 5000 | | | |
| 20053 | CHLOROPHENOLS* | | | | | | | | | | |
| 126998 | CHLOROPRENE | | | | | | | | | | |
| 1897456 | CHLOROTHALONIL | | | | | | | | | | |
| 7440473 | CHROMIUM | 10 | e | 5000 | e | | | 5000 | e | | |
| 20064 | CHROMIUM COMPOUNDS* | | | | | | | | | | |
| 7440484 | COBALT | | | | | | | | | | |
| 20075 | COBALT COMPOUNDS* | | | | | | | | | | |
| 7440508 | COPPER | | | | | | | 5000 | | | |
| 20086 | COPPER COMPOUNDS* | | | | | | | | | | |

Refer to end of table for citations

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 120718 | CRESIDINE,P | | | | | | | | | | |
| 108394 | CRESOL, M | | | | 100 | | | | 100 | | |
| 95487 | CRESOL, O | | | | 100 | | | | 100 | | |
| 106445 | CRESOL, P | | | | 100 | | | | 100 | | |
| 1319773 | CRESOL (MIXED ISOMERS) | | | | 100 | | 5000 | | 100 | | |
| 98828 | CUMENE | | | | | | 5000 | | | | |
| 80159 | CUMENE HYDROPEROXIDE | | | | | | 1000 | | | | |
| 135206 | CUPFERRON | | | | | | | | | | |
| 57125 | CYANIDE | | | | | | | | 10 | a | |
| 20097 | CYANIDE COMPOUNDS* | | | | | | | | | | |
| 110827 | CYCLOHEXANE | | | | | | 5000 | | 1000 | | |
| 4680788 | C I ACID GREEN 3 | | | | | | | | | | |
| 569642 | C.I. BASIC GREEN 4 | | | | | | | | | | |
| 989388 | C I BASIC RED 1 | | | | | | | | | | |
| 1937377 | C I DIRECT BLACK 38 | | | | | | | | | | |
| 2602462 | C I DIRECT BLUE 6 | | | | | | | | | | |
| 16071866 | C.I. DIRECT BROWN 95 | | | | | | | | | | |
| 2832408 | C I. DISPERSE YELLOW 3 | | | | | | | | | | |
| 81889 | C I. FOOD RED 15 | | | | | | | | | | |
| 3761533 | C I. FOOD RED 5 | | | | | | | | | | |
| 3118976 | C I. SOLVENT ORANGE 7 | | | | | | | | | | |
| 842079 | C I SOLVENT YELLOW 14 | | | | | | | | | | |
| 97563 | C I. SOLVENT YELLOW 3 | | | | | | | | | | |
| 128665 | C I. VAT YELLOW 4 | | | | | | | | | | |
| 94757 | D,2,4 (ACETIC ACID (2,4DICHLOR | | | | 1000 | | 1000 | | 100 | a | |
| 1163195 | DECABROMODIPHENYL OXIDE | | | | | | | | | | |
| 2303164 | DIALLATE | 100 | | | | | 5000 | | | | |
| 615054 | DIAMINOANISOLE,2,4 | | | | | | | | | | |
| 39156417 | DIAMINOANISOLE SULFATE, 2,4 | | | | | | | | | | |
| 101804 | DIAMINODIPHENYLETHER, 4,4 | | | | | | | | | | |
| 95807 | DIAMINOTOLUENE, 2,4 | 10 | | | | | 5000 | | | | |
| 25376458 | DIAMINOTOLUENE (MIXED ISOMERS) | 10 | f | | | | 5000 | a | | | |
| 334883 | DIAZOMETHANE | | | | | | | | | | |
| 132649 | DIBENZOFURAN | | | | | | | | | | |
| 96128 | DIBROMOCHLOROPROPANE (DBCB) | 1 | | | | | 1000 | | | | |
| 106934 | DIBROMOETHANE, 1,2 | 1 | | | | | 1000 | | 1000 | | |
| 95501 | DICHLOROBENZENE, 1,2 | | | | 1000 | | 5000 | | 100 | | |
| 541731 | DICHLOROBENZENE, 1,3 | | | | 1000 | | | | 100 | | |
| 106467 | DICHLOROBENZENE, 1,4 | | | | 1000 | | 5000 | | 100 | | |
| 25321226 | DICHLOROBENZENE (MIXED ISOMERS) | | | | 1000 | | | | 100 | f | |
| 91941 | DICHLOROBENZIDINE, 3,3 | 10 | | | | | 5000 | | | | |
| 75274 | DICHLOROBROMOMETHANE (BROMODICHLO | | | | | | 5000 | a | | | |
| 107062 | DICHLOROETHANE, 1,2 | 100 | a | | 1000 | | 5000 | | 5000 | | |
| 540590 | DICHLOROETHYLENE,1,2 | | | | | | | | | | |
| 75092 | DICHLOROMETHANE | | | | 1000 | a | 5000 | | 5000 | | |
| 120832 | DICHLOROPHENOL,2,4 | | | | 1000 | | 5000 | | 100 | a | |
| 78875 | DICHLOROPROPANE, 1,2 | | | | | | 5000 | | 5000 | | |
| 542756 | DICHLOROPROPYLENE,1,3 | | | | 100 | | 5000 | | 100 | | |

Refer to end of table for citations

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 62 | DICHLORVOS | | | | | | 1000 | | 10 | |
| 115 | DICOFOL | | | | | | | | | |
| 1464 | DIEPOXYBUTANE | 10 | | | | | 1000 | | | |
| 111422 | DIETHANOLAMINE | | | | | | | | | |
| 84662 | DIETHYL PHTHALATE | | | 5000 | | | 5000 | | 1000 | |
| 64675 | DIETHYL SULFATE | | | | | | | | | |
| 119904 | DIMETHOXYBENZIDINE, 3,3 | 10 | | | | | 5000 | | | |
| 57147 | DIMETHYL HYDRAZINE, 1,1 | 10 | | | | | 1000 | | | |
| 131113 | DIMETHYL PHTHALATE | 100 | e | | | | 5000 | | | |
| 77781 | DIMETHYL SULFATE | 10 | | | | | 100 | | 1000 | |
| 60117 | DIMETHYLAMINOAZOBENZENE,4 | 10 | | | | | 5000 | | | |
| 121697 | DIMETHYLANILINE,N,N | | | | | | | | | |
| 119937 | DIMETHYLBENZIDINE, 3,3 | 10 | | | | | 5000 | | | |
| 79447 | DIMETHYLCARBAMYL CHLORIDE | 1 | | | | | 5000 | | | |
| 105679 | DIMETHYLPHENOL,2,4 | | | | | | 5000 | | 100 | |
| 534521 | DINITROOCRESOL,4,6 | | | 100 | | | 100 | | 10 | |
| 51285 | DINITROPHENOL, 2,4 | | | 100 | | | 1000 | | 10 | a |
| 606202 | DINITROTOLUENE, 2,6 | 100 | | 100 | | | 5000 | | 1000 | |
| 121142 | DINITROTOLUENE,2,4 | 10 | | 100 | | | 5000 | | 1000 | |
| 117840 | DIOCTYL PHTHALATE, N | | | | | | | | | |
| 123911 | DIOXANE, 1,4 | 100 | | | | | 5000 | | 5000 | |
| 122667 | DIPHENYLHYDRAZINE, 1,2 | 10 | a | 100 | | | 5000 | | 10 | a |
| 117817 | DI(2ETHYLHEXYL) PHTHALATE | 100 | | | | | 5000 | | | |
| 84742 | DI-N-BUTYL PHTHALATE (DIBUTYL PHTHAL | | | 1000 | | | 5000 | | 10 | |
| 106898 | EPICHLOROHYDRIN | 100 | a | 100 | a | | 1000 | | 1000 | |
| 110805 | ETHOXYETHANOL, 2 | | | 1000 | | | 5000 | | 5000 | |
| 140885 | ETHYL ACRYLATE | | | | | | 5000 | | 5000 | |
| 541413 | ETHYL CHLOROFORMATE | | | | | | | | | |
| 100414 | ETHYLBENZENE | | | 5000 | | | 5000 | | 1000 | a |
| 74851 | ETHYLENE | | | | | | | | | |
| 107211 | ETHYLENE GLYCOL | | | | | | | | | |
| 75218 | ETHYLENE OXIDE | 10 | | | | | 1000 | | 1000 | |
| 96457 | ETHYLENE THIOUREA | 10 | | | | | | | 5000 | |
| 151564 | ETHYLENEIMINE (AZIRIDINE) | 1 | | | | | 100 | | | |
| 2164172 | FLUOMETURON | | | | | | | | | |
| 50000 | FORMALDEHYDE | 10 | | 100 | | | 1000 | | 1000 | |
| 76131 | FREON 113 (ETHANE, 1,1,2-TRICHLORO-1,2 | | | | | | | | | |
| 20100 | GLYCOL ETHERS | | | | | | | | | |
| 76448 | HEPTACHLOR | 1 | | | | | 1000 | | 1 | |
| 87683 | HEXACHLORO1,3BUTADIENE | 100 | | 1000 | | | 1000 | | 1 | |
| 118741 | HEXACHLOROBENZENE | 10 | | 100 | | | 5000 | | | |
| 77474 | HEXACHLOROCYCLOPENTADIENE | | | 10 | | | 5000 | | 1 | |
| 67721 | HEXACHLOROETHANE | 100 | | 1000 | | | 5000 | | 100 | |
| 1335871 | HEXACHLORONAPHTHALENE | | | | | | | | | |
| 680319 | HEXAMETHYLPHOSPHORAMIDE | | | | | | | | | |
| 302012 | HYDRAZINE | 1 | | | | | | | | |
| 10034932 | HYDRAZINE SULFATE | | | | | | | | | |
| 7647010 | HYDROCHLORIC ACID | | | | | | 5000 | | 5000 | |

Refer to end of table for citations

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 74908 | HYDROGEN CYANIDE | | | | | 100 | | 10 | a |
| 7664393 | HYDROGEN FLUORIDE | | | 100 | | 1000 | | 5000 | |
| 123319 | HYDROQUINONE | | | 1000 | | 5000 | | | |
| 78842 | ISOBUTYRALDEHYDE | | | | | | | | |
| 67630 | ISOPROPYL ALCOHOL for strong acid | | | | | | | | |
| 80057 | ISOPROPYLIDENEDIPHENOL, 4,4 | | | | | | | | |
| 7439921 | LEAD | 10 | | 1 | | 5000 | | 1 | |
| 20111 | LEAD COMPOUNDS* | | | | | | | | |
| 58899 | LINDANE (HEXACHLOROCYCLOHEXANE, GA | 10 | | | | 1000 | | 1 | |
| 108316 | MALEIC ANHYDRIDE | | | | | 5000 | | 5000 | |
| 12427382 | MANEB | | | | | | | | |
| 7439965 | MANGANESE | | | 1000 | e | | | | |
| 20122 | MANGANESE COMPOUNDS* | | | | | | | | |
| 7439976 | MERCURY | | | | | 100 | | 1 | |
| 20133 | MERCURY COMPOUNDS* | | | | | | | | |
| 67561 | METHANOL | | | | | 5000 | | 5000 | |
| 72435 | METHOXYCHLOR | | | | | 5000 | | 1 | |
| 109864 | METHOXYETHANOL, 2 | | | | | | | | |
| 96333 | METHYL ACRYLATE | | | | | | | | |
| 78933 | METHYL ETHYL KETONE | | | 1000 | | 5000 | | 5000 | |
| 60344 | METHYL HYDRAZINE | | | | | 1000 | | | |
| 74884 | METHYL IODIDE | 100 | | | | 5000 | | | |
| 108101 | METHYL ISOBUTYL KETONE | | | 5000 | a | 5000 | a | | |
| 624839 | METHYL ISOCYANATE | | | | | 100 | | | |
| 80626 | METHYL METHACRYLATE | | | 1000 | | 5000 | | 5000 | |
| 1634044 | METHYL TERTBUTYL ETHER | | | | | | | | |
| 74953 | METHYLENE BROMIDE (DIBROMOMETHANE) | | | | | 1000 | | 5000 | |
| 101144 | METHYLENEBIS(2CHLORO ANILINE) | 10 | | | | | | | |
| 101611 | METHYLENEBIS(N,N,DIMETHYL)BENZENAMIN | | | | | | | | |
| 101688 | METHYLENEBIS(PHENYLISOCYANATE) | | | | | | | | |
| 101779 | METHYLENEDIANILINE,4,4 | | | | | | | | |
| 90948 | MICHLERS KETONE | | | | | | | | |
| 1313275 | MOLYBDENUM TRIOXIDE | | | | | | | | |
| 505602 | MUSTARD GAS | 1 | | 10 | | 100 | | | |
| 91203 | NAPHTHALENE | | | | | 5000 | | 100 | |
| 134327 | NAPHTHYLAMINE, ALPHA | 100 | a | | | 5000 | | 100 | |
| 91598 | NAPHTHYLAMINE, BETA | 1 | | | | 5000 | | 100 | |
| 7440020 | NICKEL | 100 | f | 100 | | 100 | | | |
| 20144 | NICKEL COMPOUNDS* | | | | | | | | |
| 7697372 | NITRIC ACID | | | | | 1000 | | 1000 | |
| 139139 | NITRILOTRIACETIC ACID | | | | | | | | |
| 98953 | NITROBENZENE | | | | | 5000 | | 1000 | a |
| 92933 | NITROBIPHENYL,4 | | | | | | | | |
| 1836755 | NITROFEN | | | | | | | | |
| 51752 | NITROGEN MUSTARD | 10 | | | | 100 | | | |
| 55630 | NITROGLYCERIN | | | | | | | | |
| 99592 | NITROOANISIDINE, 5 | | | | | | | | |
| 88755 | NITROPHENOL,2 | | | | | 5000 | | 100 | |

Refer to of table for citations

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 100027 | OPHENOL,4 | | | | | | 5000 | | | 100 | |
| 79469 | OPROPANE, 2 | 10 | | | | | 0 | | | | |
| 55185 | ...ROSODIETHYLAMINE,N | 1 | a | | | | 00 | | | | |
| 62759 | NITROSODIMETHYLAMINE,N | 10 | a | | | | 1000 | | | | |
| 924163 | NITROSODI-n-BUTYLAMINE,N | 10 | | | | | 5000 | | | | |
| 621647 | NITROSODI-n-PROPYLAMINE,N | 10 | a | | | | 5000 | | | | |
| 156105 | NITROSODIPHENYLAMINE, P | | | | | | | | | | |
| 86306 | NITROSODIPHENYLAMINE,N | | | | | | 5000 | | | 100 | |
| 4549400 | NITROSOMETHYLVINYLAMINE,N | 10 | | | | | 1000 | | | | |
| 59892 | NITROSOMORPHOLINE,N | | | | | | | | | | |
| 759739 | NITROSO-N-ETHYLUREA,N | 1 | | | | | 5000 | | | | |
| 684935 | NITROSO-N-METHYLUREA,N | 1 | | | | | 5000 | | | | |
| 16543558 | NITROSONORNICOTINE,N | | | | | | | | | | |
| 100754 | NITROSOPIPERIDINE,N | 10 | | | | | 5000 | | | | |
| 2234131 | OCTACHLORONAPHTAHLENE | | | | | | | | | | |
| 20816120 | OSMIUM TETROXIDE | | | | | | 1000 | | | | |
| 56382 | PARATHION | | | 100 | | | 100 | | | 10 | |
| 87865 | PENTACHLOROPHENOL | | | 1000 | | | 100 | | | 10 | |
| 79210 | PERACETIC ACID | | | | | | 1000 | | | | |
| 108952 | PHENOL | | | 1000 | | | 5000 | | | 1000 | |
| 106503 | PHENYLENEDIAMINE,P | | | | | | | | | | |
| 90437 | PHENYLPHENOL, 2 | | | | | | | | | | |
| 75445 | PHOSGENE | | | | | | 10 | | | 5000 | |
| 7664382 | PHOSPHORIC ACID | | | | | | 5000 | | | 5000 | |
| 7723140 | PHOSPHORUS (YELLOW OR WHITE) | | | | | | 1000 | | | 1 | |
| 85449 | PHTHALIC ANHYDRIDE | | | | | | 5000 | | | | |
| 88891 | PICRIC ACID (2,4,6TRINITROPHENOL) | | | | | | | | | | |
| 1336363 | POLYCHLORINATED BIPHENYLS | 10 | | | | | | | | 1 | |
| 1120714 | PROPANE SULTONE | 10 | | | | | 5000 | | | | |
| 57578 | PROPIOLACTONE,BETA | 100 | | | | | 100 | | | | |
| 123386 | PROPIONALDEHYDE | | | | | | | | | | |
| 114261 | PROPOXUR (BAYGON) | | | | | | | | | | |
| 75569 | PROPYLENE OXIDE | | | | | | 5000 | | | 5000 | |
| 115071 | PROPYLENE (PROPENE) | | | | | | | | | | |
| 75558 | PROPYLENEIMINE | 1 | | | | | 1000 | | | | |
| 110861 | PYRIDINE | | | 1000 | a | | 5000 | | | 5000 | |
| 91225 | QUINOLINE | | | | | | 5000 | | | 1000 | |
| 82688 | QUINTOZENE (PENTACHLORONITROBENZEN | 100 | a | 1000 | | | 5000 | | | | |
| 81072 | SACCHARIN (MANUFACTURING) | 100 | | | | | | | | | |
| 94597 | SAFROLE | 100 | | | | | 5000 | | | | |
| 7782492 | SELENIUM | | | 100 | e | | 100 | | | 100 | e |
| 7440224 | SILVER | | | 1000 | | | 5000 | | | | |
| 20177 | SILVER COMPOUNDS* | | | | | | | | | | |
| 100425 | STYRENE | | | | | | 5000 | | | 1000 | a |
| 96093 | STYRENE OXIDE | | | | | | | | | | |
| 7664939 | SULFURIC ACID | | | | | | 1000 | | | 1000 | |
| 79345 | TETRACHLOROETHANE, 1,1,2,2 | 100 | | 1000 | | | 5000 | | | 100 | a |
| 127184 | TETRACHLOROETHYLENE (PERCHLOROETH | 100 | a | 1000 | | | 5000 | | | 1000 | |

Refer to end of table for citations

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 961115 | TETRACHLORVINPHOS | | | | | | | | | |
| 7440280 | THALLIUM | | | | | | 1000 | | | |
| 62555 | THIOACETAMIDE | 10 | | | | | | | 5000 | |
| 139651 | THIODIANILINE,4,4 | | | | | | | | | |
| 62566 | THIOUREA | 10 | | | | | 5000 | | | |
| 1314201 | THORIUM DIOXIDE | | | | | | | | | |
| 7550450 | TITANIUM TETRACHLORIDE | | | | 100 | | 100 | | | |
| 108883 | TOLUENE | | | | 1000 | | 5000 | | 1000 | a |
| 584849 | TOLUENE2,4DIISOCYANATE | | | | | | 100 | | 100 | |
| 91087 | TOLUENE2,6DIISOCYANATE | | | | | | | | | |
| 95534 | TOLUIDINE, O | 100 | | | | | 5000 | | | |
| 636215 | TOLUIDINE HYDROCHLORIDE | 100 | | | | | 5000 | | | |
| 8001352 | TOXAPHENE | 10 | | | | | 1000 | | 1 | |
| 68768 | TRIAZIQUONE | | | | | | | | | |
| 52686 | TRICHLORFON | | | | 100 | | 5000 | | 1000 | |
| 120821 | TRICHLOROBENZENE, 1,2,4 | | | | 1000 | | 5000 | | 100 | a |
| 71556 | TRICHLOROETHANE, 1,1,1 | | | | 1000 | a | 5000 | | 1000 | a |
| 79005 | TRICHLOROETHANE, 1,1,2 | 100 | a | | | | 5000 | | 1000 | |
| 79016 | TRICHLOROETHYLENE | 100 | a | | 1000 | | 5000 | | 1000 | |
| 95954 | TRICHLOROPHENOL, 2,4,5 | | | | 1000 | | 5000 | | 10 | a |
| 88062 | TRICHLOROPHENOL, 2,4,6 | 100 | | | | | 5000 | | 10 | |
| 1582098 | TRIFLURALIN | | | | | | | | | |
| 95636 | TRIMETHYLBENZENE, 1,2,4 | | | | | | | | | |
| 126727 | TRIS(2,3DIBROMOPROPYL)PHOSPHATE | 10 | | | | | 5000 | | | |
| 51796 | URETHANE (ETHYL CARBAMATE) | 100 | | | | | 5000 | | | |
| 7440622 | VANADIUM | | | | | | | | | |
| 108054 | VINYL ACETATE | | | | | | 5000 | | 1000 | |
| 593602 | VINYL BROMIDE | | | | | | | | | |
| 75014 | VINYL CHLORIDE | 1 | | | 1000 | | 100 | | 5000 | |
| 75354 | VINYLIDENE CHLORIDE (1,1 DICHLOROETHYL | 100 | a | | 1000 | | 1000 | | 5000 | |
| 108383 | XYLENE, M | | | | | | | | 1000 | |
| 95476 | XYLENE, O | | | | | | | | 1000 | |
| 106423 | XYLENE, P | | | | | | | | 1000 | |
| 1330207 | XYLENE (MIXED ISOMERS) | | | | | | 5000 | | 1000 | a |
| 87627 | XYLIDINE,2,6 | | | | | | | | | |
| 7440666 | ZINC | | | | 1000 | | | | | |
| 20199 | ZINC COMPOUNDS* | | | | | | | | | |
| 12122677 | ZINEB | | | | | | | | | |

KEY TO FOOTNOTES

All RQ values are RSG unless otherwise specified
* See individual element for data on compounds
NOTE. For metal compounds, the toxicity data presented in the table are those of the parent compound.
a = IRIS
e = WQCS
f = CURE

**Table C-3**

C – 3· CHEMICALS WITH NO REFERENCE DOSE, POTENCY FACTOR, WEIGHT OF EVIDENCE, OR REPORTABLE QUANTITY VALUES

| Jmeric Toxicity Data .or TRI Chemicals | | | |
|---|---|---|---|
| CAS | CHEMICAL | SARA CURE | HSDB |
| 60093 | AMINOAZOBENZENE, 4 | x | x |
| 6484522 | AMMONIUM NITRATE | x | x |
| 7783202 | AMMONIUM SULFATE | x | x |
| 104949 | ANISIDINE,P | | x |
| 55210 | BENZAMIDE | x | x |
| 94360 | BENZOYL PEROXIDE | x | x |
| 141322 | BUTYL ACRYLATE | x | x |
| 123728 | BUTYRALDEHYDE | x | x |
| 156627 | CALCIUM CYANAMIDE | x | x |
| 463581 | CARBONYL SULFIDE | x | ND |
| 120809 | CATECHOL (1,2 DIHYDROXYBENZENE) | x | x |
| 10049044 | CHLORINE DIOXIDE | x | x |
| 7440484 | COBALT | x | ND |
| 20075 | COBALT COMPOUNDS* | x | ND |
| 4680788 | C.I. ACID GREEN 3 | x | x |
| 569642 | C.I. BASIC GREEN 4 | x | x |
| 989388 | C.I. BASIC RED 1 | x | x |
| 2832408 | C.I. DISPERSE YELLOW 3 | x | x |
| 81889 | C.I. FOOD RED 15 | x | x |
| 3118976 | C.I. SOLVENT ORANGE 7 | x | x |
| 842079 | C.I. SOLVENT YELLOW 14 | x | x |
| 97563 | C.I. SOLVENT YELLOW 3 | x | x |
| 128665 | C.I. VAT YELLOW 4 | x | x |
| 334883 | DIAZOMETHANE | x | x |
| 132649 | DIBENZOFURAN | x | x |
| 111422 | DIETHANOLAMINE | x | x |
| 64675 | DIETHYL SULFATE | x | x |
| 541413 | ETHYL CHLOROFORMATE | x | x |
| 74851 | ETHYLENE | x | x |
| 1335871 | HEXACHLORONAPHTHALENE | x | x |
| 680319 | HEXAMETHYLPHOSPHORAMIDE | x | x |
| 78842 | ISOBUTYRALDEHYDE | x | x |
| 67630 | ISOPROPYL ALCOHOL for strong acid | x | x |
| 80057 | ISOPROPYLIDENEDIPHENOL, 4,4 | x | |
| 101688 | METHYLENEBIS(PHENYLISOCYANATE) | x | x |
| 1313275 | MOLYBDENUM TRIOXIDE | x | x |
| 92933 | NITROBIPHENYL,4 | x | x |
| 55630 | NITROGLYCERIN | x | x |
| 2234131 | OCTACHLORONAPHTAHLENE | x | x |
| 88891 | PICRIC ACID (2,4,6TRINITROPHENOL) | x | x |
| 123386 | PROPIONALDEHYDE | x | x |
| 115071 | PROPYLENE (PROPENE) | x | x |
| 7664939 | SULFURIC ACID | x | x |
| 1314201 | THORIUM DIOXIDE | x | x |
| 68768 | TRIAZIQUONE | x | ND |
| 95636 | TRIMETHYLBENZENE, 1,2,4 | x | x |
| 87627 | XYLIDINE,2,6 | x | x |

# Appendix D

## Review of Data Sources

## Appendix D - Review of Data Sources

| Database or Listing | Purpose of Data | Types of Information | Number of TRI Chemicals* | Format or Access |
|---|---|---|---|---|
| Health Effects Database (HEDB) | Integration of data from existing EPA databases. | Includes reportable quantities, threshold planning quantities, indicators of carcinogenicity, oral reference dose. | 312 | dBASE file for PC use. |
| Roadmaps | Assist non-EPA users who assess TRI chemicals. | Primarily a directory of sources of information on individual chemicals. Also provides reportable quantities and measures of exposure limits. | 312 | PC software |
| Integrated Risk Information System (IRIS) | Designed for EPA decision-making and regulatory activities; represents EPA risk information consensus. | Includes measures of chronic health hazards, carcinogenicity, reportable quantities, water quality criteria, and maximum contaminant levels. | 200+ | ASCII files via E-mail or Toxnet |
| Risk Screening Guide Appendix A ("PRETOX" data) | Toxicology data to support TRI Risk Screening Guide. | Contains various indicators of toxicity, including reportable quantities, RfDs and Water Quality Criteria. | 309 | dBASE file for PC use. |
| Hazardous Substances Data Bank (HSDB) | Designed to provide a single source of broad toxicological and pharmacological information on chemical substances. | Includes both toxicological effects from scientific literature as well as regulatory standards. Also includes environmental fate and exposure potential. Information on over 4,100 substances in total. | Unknown | On-line mainframe through NLM TOXNET |

| Database or Listing | Purpose of Data | Types of Information | Number of TRI Chemicals* | Format or Access |
|---|---|---|---|---|
| AQUIRE - Aquatic Toxicity Retrieval System | Source of quick access to comprehensive, systematic aquatic toxicity data. | Indexes the conditions and results of scientific studies; provides lethal and effect concentrations and bioconcentration factors for aquatic systems. | unknown | PC or mainframe software |
| U.S. Census Data | Used at EPA to support exposure assessments. | Includes 1980 U.S. Census population data and 1983 estimates, encoded by block group/enumeration district centroids. | N/A | On GEMS (VAX) and PC-GEMS |
| REACH Data; REACHSCAN Data. | Used at EPA to support exposure assessments. | Includes stream reach location information; REACHSCAN allows identification of downstream water intakes. | N/A | On GEMS (VAX) and PC-GEMS |
| Federal Reporting Data System (FRDS) | Used at EPA to support exposure assessments, drinking water analyses. | Includes public water supply system data, including location, volume, source, and population served. | N/A | On GEMS system (VAX) |

* There are a total of 317 TRI chemicals.

# Appendix E

## Waste Volumes by Industry

Table 4-7 NUMBER OF LANDFILLS BY AMOUNT OF WASTE RECEIVED IN 1984

| Waste Type | Survey Response Rate | Quantity of Waste Received | | | Total Landfills Per Waste Type* |
|---|---|---|---|---|---|
| | | < 30,000 cu yds (< 30 tons/day) | 30,000-600,000 cu yds (30-500 tons/day) | > 600,000 cu yds (> 500 tons/day) | |
| Municipal Solid Waste | 85% | 5,309 (67%) | 2,211 (28%) | 408 (5%) | 7,925 (100%) |
| Industrial Waste | 82% | 2,289 (79%) | 523 (18%) | 72 (2.5%) | 2,884 (100%) |
| Demolition Waste | 83% | 1,608 (75%) | 468 (22%) | 78 (3.6%) | 2,154 (100%) |
| Other Waste | 85% | 790 (93%) | 51 (6%) | 11 (1.3%) | 852 (100%) |

SOURCE: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

* Percentages may not total 100 percent because of rounding.

Table 4-9. NUMBER OF INDUSTRIAL ESTABLISHMENTS WITH LANDFILLS BY ANNUAL WASTE QUANTITY DISPOSED IN THEM IN 1985

| Industry Type | Number of Establishments by Annual Quantity of Waste Disposed of in Landfills in 1985 (thousand tons) | | | | | | |
|---|---|---|---|---|---|---|---|
| | Less than 0.5 | 0.5-5 | 5.1-20 | 21-100 | 101-1,000 | More than 1,000 | Total Establishments Per Industry Type[a] |
| Organic Chemicals | 2 | 4 | 4 | 2 | 1 | 0 | 13 |
| Primary Iron and Steel | 69 | 55 | 29 | 13 | 9 | 0 | 176 |
| Fertilizer & Agricultural Chemicals | 25 | 2 | 0 | 0 | 2 | 1 | 30 |
| Electric Power Generation | 23 | 13 | 6 | 23 | 57 | 3 | 126 |
| Plastics and Resins Manufacturing | 18 | 6 | 2 | 2 | 0 | 0 | 28 |
| Inorganic Chemicals | 30 | 31 | 10 | 9 | 0 | 1 | 81 |
| Stone, Clay, Glass, & Concrete | 873 | 129 | 85 | 46 | 10 | 0 | 1,143 |
| Pulp and Paper | 26 | 14 | 83 | 44 | 12 | 0 | 179 |
| Primary Non-ferrous Metals | 32 | 35 | 7 | 13 | 2 | 0 | 90 |
| Food and Kindred Products | 127 | 22 | 17 | 12 | 11 | 0 | 189 |
| Water Treatment | 33 | 33 | 0 | 3 | 0 | 0 | 69 |
| Petroleum Refining | 21 | 9 | 8 | 1 | 1 | 0 | 40 |
| Rubber and Misc. Products | 2 | 22 | 2 | 10 | 0 | 0 | 36 |
| Transportation Equipment | 37 | 8 | 7 | 7 | 1 | 0 | 54 |
| Selected Chem. and Allied Products | 6 | 6 | 6 | 1 | 0 | 0 | 19 |
| Textile Manufacturing | 12 | 6 | 7 | 0 | 0 | 39 | 25 |
| Leather and Leather Products | 8 | 0 | 1 | 0 | 0 | 0 | 9 |
| Total[a] | 1,344 | 396 | 274 | 181 | 105 | 5 | 2,305[b] |

SOURCE: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

a These are the correct totals. Table entries may not add to their respective totals due to rounding.

b Overall response rate for this table is 99.3 percent.

Table 4-62. NUMBER OF ESTABLISHMENTS WITH SURFACE IMPOUNDMENTS BY INDUSTRY AND WASTE QUANTITY DISPOSED OF IN THEM IN 1985

| Industry Type | Number of Establishments by Waste Quantity Disposed of in Them in 1985 (tons) | | | | | | | | Total Establishments Per Industry Type[a] |
|---|---|---|---|---|---|---|---|---|---|
| | Less Than 3 | 3-9 | 10-99 | 100-499 | 500-999 | 1,000-4,999 | 5,000-10,000 | Greater Than 10,000 | |
| Organic Chemicals | 1 | 2 | 2 | 12 | 1 | 11 | 13 | 45 | 86 |
| Primary Iron and Steel | 1 | 1 | 37 | 18 | 3 | 24 | 10 | 89 | 182 |
| Fertilizer and Agricul Chemicals | 3 | 1 | 37 | 9 | 3 | 6 | 3 | 47 | 110 |
| Electric Power Generation | 5 | 3 | 29 | 29 | 7 | 20 | 7 | 207 | 306 |
| Plastics and Resins Manufacturing | 3 | 2 | 4 | 6 | 1 | 8 | 2 | 50 | 77 |
| Inorganic Chemicals | 3 | 1 | 25 | 34 | 14 | 83 | 32 | 145 | 340 |
| Stone, Clay, Glass, and Concrete | 42 | 106 | 419 | 594 | 194 | 217 | 76 | 290 | 1,939 |
| Pulp and Paper | 9 | 23 | 0 | 29 | 3 | 19 | 15 | 201 | 301 |
| Primary Nonferrous Metals | 6 | 5 | 38 | 18 | 2 | 51 | 10 | 55 | 186 |
| Food and Kindred Products | 13 | 30 | 105 | 215 | 54 | 353 | 129 | 799 | 1,700 |
| Water Treatment | 0 | 0 | 34 | 34 | 5 | 17 | 32 | 207 | 329 |
| Petroleum Refining | 30 | 4 | 60 | 12 | 10 | 70 | 8 | 117 | 310 |
| Rubber and Miscellaneous Products | 41 | 1 | 22 | 1 | 10 | 1 | 3 | 46 | 126 |
| Transportation Equipment | 7 | 0 | 19 | 29 | 2 | 9 | 8 | 44 | 118 |
| Selected Chemicals and Allied Products | 2 | 0 | 2 | 3 | 4 | 4 | 5 | 33 | 52 |
| Textile Manufacturing | 1 | 16 | 39 | 1 | 11 | 21 | 16 | 283 | 388 |
| Leather and Leather Products | 0 | 0 | 3 | 3 | 1 | 0 | 1 | 18 | 27 |
| Total[a] | 168 | 197 | 877 | 1,049 | 325 | 916 | 369 | 2,677 | 6,578[b] |

SOURCE: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States. Volume 1, Draft Final (Revised), April 15, 1988.

a These are the correct totals. The table entries may not add to their respective totals because of rounding.

b Overall response rate for this table is 98.5 percent.

Table 4-83. NUMBER OF ESTABLISHMENTS WITH WASTE PILES BY INDUSTRY TYPE AND WASTE QUANTITY DISPOSED OF IN THEM IN 1985

| Industry Type | Number of Establishments According to Amount of Waste Disposed in Them (thousand tons) | | | | | | Total Establishments Per Industry Type[a] |
|---|---|---|---|---|---|---|---|
| | Less than 0.5 | 0.5-5 | 5.1-20 | 21-100 | 101-1,000 | More than 1,000 | |
| Organic Chemicals | 21 | 15 | 2 | 0 | 0 | 0 | 37 |
| Primary Iron and Steel | 202 | 74 | 24 | 14 | 2 | 2 | 317 |
| Fertilizer and Agricultural Chemicals | 19 | 2 | 4 | 1 | 3 | 1 | 30 |
| Electric Power Generation | 77 | 8 | 0 | 8 | 1 | 0 | 93 |
| Plastics and Resins Manufacturing | 19 | 1 | 2 | 0 | 0 | 1 | 23 |
| Inorganic Chemicals | 30 | 12 | 4 | 2 | 7 | 4 | 60 |
| Stone, Clay, Glass, and Concrete | 1,549 | 184 | 131 | 57 | 21 | 0 | 1,942 |
| Pulp and Paper | 51 | 63 | 38 | 7 | 2 | 0 | 162 |
| Primary Non-ferrous Metals | 198 | 41 | 14 | 4 | 3 | 1 | 261 |
| Food and Kindred Products | 297 | 28 | 4 | 11 | 0 | 0 | 340 |
| Water Treatment | 41 | 1 | 0 | 0 | 0 | 0 | 42 |
| Petroleum Refining | 112 | 21 | 2 | 0 | 0 | 0 | 135 |
| Rubber and Miscellaneous Products | 76 | 21 | 1 | 0 | 0 | 0 | 98 |
| Transportation Equipment | 213 | 70 | 15 | 2 | 1 | 0 | 300 |
| Selected Chemicals and Allied Products | 33 | 6 | 0 | 0 | 0 | 0 | 39 |
| Textile Manufacturing | 90 | 10 | 0 | 0 | 0 | 0 | 99 |
| Leather and Leather Products | 37 | 3 | 0 | 0 | 0 | 0 | 39 |
| Totals | 3,064 | 558 | 242 | 106 | 40 | 9 | 4,019[b] |

SOURCE: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

a These are the correct totals. The table entries may not add to their respective totals because of rounding.

b Overall response rate for this table is 95.6 percent.

# Appendix F

## *Options for Indicator Computation and Normalization*

## I. Options for Indicator Computation

The TRI indicator will be calculated by combining the individual scores of the TRI chemical-facility-media components. Each component's value is related to a chemical's risk to either human health or the environment (depending on the indicator). The value is calculated based on measures of the volume of release from a facility, the chemical's toxicity, and the potential exposed population for the media of release.

This appendix discusses the two leading methodologies considered for calculating the TRI indicator. The method of calculation will influence the ways we can adjust the indicator and how the indicator will change in response to the adjustments as facilities and chemicals are added over time.

**Simple Sum of the Component Scores:**

$$I = S_1 + S_2 + S_3 + \ldots + S_n$$

where:

I = TRI indicator
S = facility-chemical-medium-specific subindicator

In this method, each component score makes a contribution proportional to its size. Simply, it is the total "risk" resulting from all chemical-facility-media releases. It should be noted that subscores for particular chemicals, industries, and regions can also be calculated for indicator diagnostics.

**Simple Sum Normalized to a Base Year:**

$$I = \frac{(S_1 + S_2 + S_3 + \ldots + S_n)_{present\ year}}{(S_1 + S_2 + S_3 + \ldots + S_n)_{base\ year}} \cdot 100\%$$

Like the simple sum method, this method represents each component score proportionately. Its primary advantage is that it is a dimensionless ratio that tracks progress over time and continuously looks back at the beginning of the indicator record. A score of 60 indicates that the overall chemical-facility-media risk has been reduced by 40 percent since the TRI indicator began. Hence, each individual score has meaning, as does the change from year to year.

Other Methods of Calculation

We considered alternative means of calculating the indicator. Some of these included the arithmetic mean of the component scores, the geometric mean of the scores, and the least-square difference of the scores. Although each of these methods generates a score that will fluctuate as the individual components of the risk, the methods do not produce readily interpretable results.

For the greatest sensitivity in the actual indicator score, as well as for the greatest ease in calculation and interpretation, we recommend that the chemical-facility-media scores simply be added and then adjusted to a manageable level.

## II. Normalizing the Indicator

This section discusses options considered for modifying the indicator to accommodate the addition of SIC codes and chemicals for TRI reporting purposes. We discuss how the failure to report chemical release data as well as data errors can affect the calculation of the indicator. We also present an example to illustrate both the necessity of designing a method of normalization and the implications of the methods presented here.

As discussed previously, the indicator should be designed to accommodate an increase in the number of components of the TRI. This increase can occur through any of three mechanisms: an addition of chemicals to the TRI list, an increase in the number of facilities by enhancing the SIC code list, and an increase in facility compliance with existing reporting requirements. Each of these scenarios enhances the accuracy of the report because they supply missing information. However, this addition changes the scope of the indicator (from a small subset to a larger subset), thereby limiting the effectiveness of comparison between current and past values.

The addition to or deletion of chemicals from the TRI roster will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. The deletion of chemicals will presumably have a minor effect since such chemicals would be deleted due to their low risk; by definition these chemicals will make only a minimal contribution to the indicator. Deletion will most likely occur in batches every few years. The addition of SIC codes will likely follow investigations of the TRI chemicals revealing other industries that emit the listed chemicals. Compliance could also in the future. In 1989, the Office of Toxic Substances studied compliance with TRI reporting requirements. The study found that the compliance rate was 81.7 percent in the first year of reporting. Follow up studies have not been done to determine the improvement in compliance with Section 313. However, the OTS study stated that under full compliance, the estimated number of respondents would be over 29,000. In the last two years of reporting, the number of reporting facilities has not approached that figure, despite a lowering of reporting thresholds.

The fundamental problem in maintaining a single, continuous indicator is that there is no way to differentiate between fluctuations due to changes in actual environmental risk and those due to changes in the chemical or facility roster. Therefore, to maintain the integrity of the indicator when chemicals are added to the roster, each addition to the indicator should be accompanied by some kind of adjustment. Methodologies for accommodating the addition of chemical-facility-media components are presented below along with discussions of their impact on the accuracy of the indicator. First, we present a hypothetical example of indicator values over a five year period and then articulate a number of options for normalizing the index.

Example:

The calculation of the indicator begins in 1988, and we select the Simple Sum method of calculating the indicator. For the first 5 years the indicator scores are as follows:

| Year | Indicator Score |
|---|---|
| 1988 | 1,000 |
| 1989 | 950 |
| 1990 | 850 |
| 1991 | 800 |
| 1992 | 775 |

In 1993, the Agency adds another 200 chemicals to the TRI list as well as five SIC codes. The 1993 score of the original set of TRI chemicals and SIC codes is 750, meaning that the risks associated with those chemicals and facilities have decreased. The score for the additional set of chemicals and facilities is 500.

Do Nothing

The Do-Nothing scenario is important to examine since the benefits of lost continuity may outweigh the disadvantages and the effort required to work around them. For this method, the score will rise when components are added and will no longer describe the environmental progress as compared to the previous roster. In our example, the indicator score will read 775 in 1992 and 1,250 in 1993. It will be impossible to recalculate the previous years' scores with the new chemicals because release data will not be available. Thus, information on progress since the initial roster will be lost.

The Do-Nothing scenario could be viewed as a more accurate representation of the "complete picture" of environmental risk. If, for example, the indicator score for the universe of all chemicals and all facilities were actually 4,000, and this initial TRI setup

provides a score of 1,000, then the subsequent addition of components to the TRI will fill in the additional 3,000 points for which no information exists. Yet for the public to understand the severity of a change, increases in the indicator score from new chemicals ought to occur on the same scale as that of the original set. As discussed earlier, the public will perceive the indicator score presented with the first set of TRI chemicals and facilities as representing the risk associated with all chemicals and facilities. The public will believe that the new score of 1250 means that the risks posed to them have risen by 475 points; actually, the risk to them has not increased at all, they are just better represented. An increase in the number of components should not actually increase risk but should redistribute the individual contributions to the total risk.

**Creation of a Separate Indicator**

Chemicals could be added to the TRI roster one or two at a time each year or in a large number once every five years. If the latter occurs exclusively, we could establish an indicator consisting solely of the new chemicals and allow the scores of the old indicator to continue as before. In our example, the TRI indicator would be reported as two scores: in 1993 it would be 750 for the original set of TRI chemicals and facilities and 500 for the new set of chemicals and facilities. This approach has two advantages. First, this system could accurately track the progress of the original roster as well as the new roster. Second, the indicator for each roster could be compared and the program could establish priority for alleviating environmental problems associated with the new or old list.

The primary disadvantage of two indicators is the loss of a single instrument. Chemicals and SIC codes will be added to the TRI more than once, and each time another four indices (human health and environmental risk; chronic and acute effects) will be needed. Each of these indices is also compared at regional, state and local levels. Maintaining a number of indicators will create public confusion, as people try to keep track of each separate indicator change from the previous year. A second disadvantage follows from the Do-Nothing scenario: if people add these scores together to get the "total" score, they will perceive an increase in overall risk. Finally, if TRI chemicals are added continuously in small amounts, this method will be extraordinarily difficult to implement as new indices are created each year.

**Ratio Adjustment**

The ratio adjustment method is used with the Dow Jones Industrial Average, the Producer Price Index, the Consumer Price Index, and the New York Stock Exchange Composite Index. The underlying components of each of these indices are updated periodically to reflect fundamental shifts in what is being measured. For example, this year the Dow substituted three service sector stocks for three industrial stocks to reflect the U.S. economy's shift toward the service sector. The Producer and Consumer Price indices revise their basket of goods decennially to reflect the caprice of consumer taste. The NYSE

Composite Index, which encompasses every stock on the New York Stock Exchange, is revised every time companies start up, merge, or fail.

The adjustment is straightforward. On the first day that the revised components are employed, the index is calculated twice, once based on the old components and again based on the revised components. Thereafter, the ratio between these two index values is used to adjust the index as it is calculated from the revised components:

$$I = I_{\text{revised components}} \cdot \frac{I_{\text{old, last day}}}{I_{\text{new, first day}}}$$

In our example, the old system yielded a score of 750 and the new system yields a score of 1,250. To scale down the new score to maintain continuity, we multiply the new score by (750/1,250) = 0.6. All subsequent scores (1994, 1995, and so on) will also be calculated in the same manner and then multiplied by 0.6, until another addition requires the determination of another multiplication factor.

One disadvantage of this method is the loss of information concerning the original set of chemicals and facilities in the presentation of one indicator that integrates all scores. Even if the indicator publishes the scores associated with each set of chemicals, the scale will have changed, prohibiting direct comparison. (Compare this to the method where original and supplemental indices are both tracked.)

Another disadvantage is the misrepresentation of the behavior of the new set of chemicals and facilities. The TRI indicator is distinct from the Dow in a way that affects the applicability of this system. The Dow uses a few stocks to model the entire market and assumes that the behavior of these stocks reflects the general behavior of all stocks. This implies that substitution of one stock for another in the Dow fits conceptually with its purpose. The TRI indicator seeks to reflect the levels of risk to human health and the environment by including a subset of the universe of all chemicals and facilities. The behavior of risks posed by all chemicals and facilities cannot be said to match the behavior of the set of TRI chemicals and facilities. The inclusion in TRI focuses a facility's attention upon particular chemicals and presumably results in changes of releases of TRI chemicals by TRI facilities. By fitting the combined score of new and old TRI chemicals and facilities to the score of the old, we inherently assume that the new have experienced reductions in risk identical to the old. In truth, we have no way of knowing the past pattern of releases for new additions. Emissions may have not changed at all since these chemicals have not yet been targeted by TRI; on the other hand, emissions may have been reduced more than emissions of old TRI chemicals because the new chemicals may have already been regulated by certain EPA programs or by states, or companies may have reduced emissions voluntarily.

## Normalization to a Base Level

This method reflects the Do-Nothing approach except for taking necessary adjustments for the use of normalization. Instead of using the score resulting from a base year, base levels could be used, defined as the sum of the component scores at the first year that each list is added to the TRI Indicator. For example, upon the first addition to the TRI (combining the initial roster, list 1, and the addition, list 2), the indicator could be calculated as follows:

$$I = \frac{(S_1 + S_2 + \ldots + S_m + \ldots + S_n)_{present\ year}}{(S_1 + S_2 + \ldots + S_m)_{first\ year\ of\ list\ 1} + (S_{m+1} + \ldots + S_n)_{first\ year\ of\ list\ 2}}$$

where:

S = each chemical-facility-media component score,
n = total number of TRI chemicals,
m = number of TRI chemicals in the first list, and
m-n = number of chemicals added to the roster.

Following the example, the score for 1988 would be (1,000/1,000)*100 = 100. The following scores would be (950/1,000) = 95, (850/1,000) = 85, (800/1,000) = 80, and (775/1,000) = 77.5. In 1993, the score would be calculated as follows:

$$\frac{750 + 500}{1000 + 500} = 83.3$$

While this score represents an increase, it is not as drastic as using the simple sum method, and it can be explained to the public as resulting from the addition of TRI chemicals and facilities to the indicator. This equation can also be used to indicate relative percentages of the two different sets of chemicals and facilities (750/1,500 = 50 for the original and 500/1,500 = 33.3 for the new). However, as with ratio adjustment, the original set cannot be said to have improved by (77.5 - 50) = 27.5 points.

## Variations on the Previous Methods

Improvements in the way in which the smaller TRI chemical universe models the larger one would lead to more meaningful comparisons between the old and new indices. One way to improve this modeling ability is to employ data on the new chemicals for the

period predating their addition to TRI. If we had the release data, we could calculate exactly how inaccurate the small TRI chemical universe was as a model and adjust it accordingly. Although these data will not exist except as part of a state inventory, we could approximate them through the correlation of releases of other chemicals. For example, if a facility reports the release of a chemical because of its addition to the TRI, it is very likely that the chemical had been released at that level all along. A rough approximation would be to look at changes in releases from that facility and then correlate the release of the new chemical in back years.

Yet another possibility is to combine more than one of the above examples. For example, it may be appropriate to maintain one "primary" indicator score while also maintaining "subscores" for each of the sets of TRI chemicals (i.e., the original set and each additional set). The main score could be calculated using the simple sum and normalized with the ratio adjustment each time an additional set of chemicals is added. The subscores could be calculated for each set of TRI chemicals using the normalization to a base year; each of these subscores could be maintained separately. In our example, after the addition of chemicals, the main indicator score would be 750 while the subscores would be (750/1,000) = 75 and (500/500) = 100. As in the discussion of the creation of separate indices, this combination depends upon the addition of TRI chemicals in large groups every number of years. If routine additions occur, the main indicator could be calculated as above and only one subscore, that of the original set of chemicals, could be maintained.

**Start Over**

The last system that may be used is to announce the beginning of a new indicator. Once every 5 years the Agency could integrate all of the additions to and deletions from TRI that had occurred since the beginning of the previous indicator. EPA could announce that to better assess the risks to the environment posed by chemical releases, certain chemicals have been deleted or added based upon TRI criteria and that a new indicator, calculated in the same manner at the same scale, has begun. It is also quite possible that experience with the indicator may suggest a new mode of calculation by the time more chemicals and facilities are ready to be added.

# Appendix G

## Understanding the TRI Indicator Modelling Approach

## I. PURPOSE OF THE INDICATOR

The purpose of the indicator is to track changes in environmental and human health risk over time. The calculation of the indicator requires consideration of release volume, toxicity, exposure potential and population exposed.

In our method, the indicator will be calculated as the sum of facility-, chemical-, and medium-specific subindicators:

- Each non-zero chemical release, facility, and media combination present in the TRI will have a calculated subindex based on toxicity, exposure, and uncertainty.

- Using subindexes allows disaggregation of the total index value into groupings of interest for analysis or to facilitate explanation of interior index fluctuations. Pinpointing areas of change is built into the indicator algorithm.

## II. BASIC STEPS

For each facility, *j*, and each chemical released at that facility, *k*, a medium-specific subindex will be calculated. These are the most elemental components of the index and can be summed in innumerable ways to view a desegregated TRI indicator to ease analysis and explanation of change. The basic subindex calculation is:

1. Locate facility

   for direct releases: locate TRI reporting facility
   for transfers: match TRI transfer to a receiving facility, then locate receiving facility

2. Match geographic and demographic features to location

   the key to this step will be the use of the BGREACH grid

3. Estimate environmental concentration

   the text of the report explains particular models and methods used for each pathway

4. Calculate dose, then assign exposure potential score based on dose

   exposure potential scoring system presented in report; it is based on calculated dose and uncertainty category

5. Weight exposure potential by toxicity and population scores

   toxicity and population scoring matrices presented in report

## III. PATHWAY BY PATHWAY ALGORITHMS

### AIR RELEASES

1. Locate facility

   - Locate facility via longitude/latitude from TRI.

2. Match geographic and demographic features to location

   - Match TRI facility location to BGREACH grid cell

3. Estimate population-weighted environmental concentration

   - Convert lbs/yr release estimate in TRI to grams/sec.
   - Calculate concentration in the nearest 100 cells (10 $km^2$) based on ISCLT equations for stack or fugitive sources.
   - Weight calculated concentrations by population in each cell to arrive at population-weighted average concentration.

4. Calculate dose, then assign exposure score.

   - Convert concentration to dose using inhalation rate, body weight. Assign score using matrix and uncertainty category A.

5. Multiply exposure potential by toxicity score and population score

   - Multiply exposure score by population (population of nearest 100 cells rounded to the nearest 1000; if less than 1000, use 1000), adjusted for uncertainty.

   - Multiply result by toxicity score to arrive at final facility-chemical-air specific subindex $I_{j,k,air}$

## WATER RELEASES

1. Locate facility

   - Locate facility via longitude/latitude from TRI.

2. Match geographic and demographic features to location

   - Match TRI facility location to BGREACH grid cell

3. Estimate population-weighted environmental concentration

   - Determine initial concentration from reported TRI water discharge and water volume in cell. If cell contains no water volume information (e.g., cell contains no water body), find nearest cell with water body and assume facility releases at that point.

   - Calculate water concentration in each cell through which water body flows (defined by $NEXT_{xy}$ values) using the decay equation and volume and speed information. Using chemical-specific BCF values, also calculate the fish concentration in each cell.

4. Calculate dose, then assign exposure score based on dose and uncertainty category A.

   For drinking water pathway:

   - If cell contains a drinking water intake, convert water contaminant concentration in cell to dose using drinking water intake rate

   - Weight dose in cell served by the size of the population served in the cell

   - Continue traversing the water body through cells and checking for drinking water intakes, until water body is completely traversed or contaminant is reduced to negligible levels

   - Derive average dose by dividing the weighted doses by total population served by all cells with intakes

For fish ingestion pathway:

- In all cells, convert fish contaminant concentration to dose using fish ingestion rate and body weight
- Weight dose in cell by the number of persons living in the cell who fish
- Continue traversing the water body through cells until water body is completely traversed or contaminant is reduced to negligible levels
- Derive average dose by dividing the weighted doses by total fishing population in all cells

For drinking water pathway, assign exposure score using matrix and uncertainty category B. For fish ingestion pathway, assign exposure score using matrix and uncertainty category C.

5. Weight exposure score by toxicity score and population score

- Multiply drinking water exposure score by population size (rounded to nearest 1000), adjusted by uncertainty category B
- Multiply fish ingestion exposure score by population size (rounded to nearest 1000), adjusted by uncertainty category C
- Multiply result by toxicity score to arrive at final facility-chemical-water specific subindex $I_{j,k,wat}$.

LAND RELEASES

1. Locate facility

   - Locate facility via longitude/latitude from TRI.

2. Match geographic and demographic features to location

   - Match TRI facility location to BGREACH grid cell

3. Estimate environmental concentration

   - Determine if site is regulated by RCRA. If form reports RCRA ID number, assume no exposure.

   - If form does not report RCRA ID number, determine concentration in leachate based on equations in text.

   - Apply the dilution and attenuation factor (DAF) to arrive at well concentration.

4. Calculate dose, then assign exposure score based on dose and uncertainty

   - Convert concentration to dose using water ingestion rate, body weight, and uncertainty category C

5. Weight exposure score by toxicity and population scores

   - Using the WELL variable in the BGREACH file, estimate the number of well drinkers in the 4 nearest cells (2 $km^2$); adjust by uncertainty category C and multiply result by the exposure score.

   - Multiply this result by the toxicity score to arrive at the facility-chemical-groundwater subindex, $I_{j,k,groundwater}$

POTW DISCHARGES

1. Locate facility

   - Match DCN (TRI Document Control Number) to the POTW file to determine the POTW zip code.

   - Locate POTW on using the longitude and latitude of the center of the zip code areas in which the POTW is located.

2. Match geographic and demographic features to location

   - Match POTW facility location to BGREACH grid cell

3. Estimate environmental concentration

   - Determine, based on chemical specific removal rates, amount of contaminant removed by treatment at the POTW.

   - Use the amount removed as a direct discharge to water in the surface water body receiving the POTWs effluent and follow procedure for water discharges above. If the POTWs cell does not contain a water body, find the nearest water body to the cell and assume POTW releases at that point

   - From the amount not removed, use partition rates to determine amount of contaminant that volatilized and the amount in sludge

Step 4 (calculate dose, then assign exposure potential score based on dose) and step 5 (weight exposure potential by toxicity and population scores) are performed as appropriate, depending on the environmental compartment into which the chemical partitions:

   - Volatilized contaminant is modelled following the procedure for air releases above.

   - Contaminated sludge is modelled by using methods appropriate to disposal practice (if such a match can be made) or by using a chemical-specific unit exposure from national assessment of exposures from disposal of municipal sludge.

OFFSITE TRANSFERS

1. Locate facility

   - Match DCN (Document Control Number) to the OFFSITE file to determine the off-site facility zipcode.

   - Locate off-site facility by using the longitude and latitude of the center of the zipcode area.

2. Match geographic and demographic features to location

   - Match location of off-site facility to BGREACH cell

3. Estimate environmental concentration

   - Based on the treatment code reported by the facility, model either incinerators or land disposal (underground injection?). If transferred to a RCRA facility, assume no risk. Otherwise:

   - For incinerators, apply a chemical-specific incinerator efficiency and model remaining release following the procedure for direct air releases.

   - Land disposal is modeled in the same way as on-site landfilling with the exception of the addition of volatilized chemical consideration. Emission of volatilized chemicals will be estimated using equations in Chapter 5, and then modelled following the procedure for direct fugitive air releases.

Step 4 (calculate dose, then assign exposure potential score based on dose) and step 5 (weight exposure potential by toxicity and population scores) are performed as appropriate, depending on the treatment method.

The results of the incinerator results or the result of the sum of the groundwater and volatilization results becomes the facility-chemical-offsite subindicator, $I_{j,k,OFFSITE}$.

## IV. ADDING IT ALL UP

A total score for the facility may be calculated by adding all of its subindicators for all chemicals it releases (K = 1 to n):

$$I_J = \sum_{K=1}^{n} (I_{k,air} + I_{k,water} + I_{k,groundwater} + I_{k,POTW} + I_{k,offsite})$$

A total score for a chemical may be calculated by adding all subindicators calculated for that chemical at any releasing facility (J = 1 to m):

$$I_K = \sum_{J=1}^{m} (I_{J,air} + I_{J,water} + I_{J,groundwater} + I_{J,POTW} + I_{J,offsite})$$

and:

$$\sum I_J = \sum I_K = \textit{OVERALL TRI INDICATOR}$$