

United States Environmental Protection Agency Office of Pollution Prevention and Toxics Washington, DC 20460

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# EPA's Risk-Screening Environmental Indicators (RSEI) Chronic Human Health Methodology

**RSEI** Version 2.1

### Acknowledgments

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# **Executive Summary**

## **ES-1.** Introduction

EPA's Risk-Screening Environmental Indicators (RSEI) is a screening-level tool that assesses the potential impact of industrial releases from pounds-based, hazard-based, and risk-related perspectives. RSEI uses risk concepts to quickly and easily screen large amounts of data, saving time and resources. RSEI is particularly useful for examining trends to measure change, ranking and prioritizing chemicals and industry sectors for strategic planning, conducting risk-related targeting, supporting community-based projects, and investigating environmental justice issues.

Using estimates of pounds of chemical releases to investigate potential health and environmental impacts is limited by the assumptions that all chemicals are equally toxic and all people are equally exposed. Formal risk assessments are more accurate, but are complicated and time consuming to prepare, requiring detailed data which is not always available, and the results are often limited in scope and geographic area. The RSEI approach augments estimates of pounds released with toxicity and exposure considerations, but does not address all of the potential factors that a full risk-assessment would include.

RSEI considers the following information: the amount of chemical released, the toxicity of the chemical, its fate and transport through the environment, the route and extent of human exposure, and the number of people affected. This information is used to create numerical values that can be added and compared in limitless ways to assess the relative risk of chemicals, facilities, regions, industries, or many other factors. The values are for comparative purposes and only meaningful when compared to other values produced by RSEI. It should be emphasized that the result is *not* a detailed or quantitative risk assessment, *but offers a screening-level, risk-related perspective for relative comparisons of chemical releases.* 

The RSEI approach is very flexible and can be implemented in various ways. The use of the model is not limited to any specific set of chemicals; in principle, the adaptable method can model any chemical if toxicity characteristics, physicochemical properties, release levels, and release location are known or can be estimated. RSEI is currently implemented as the RSEI Chronic Human Health model, which addresses chronic human health effects and chronic exposures, and uses estimates of annual releases from EPA's Toxics Release Inventory (TRI).

As an indication of improvements in environmental quality over time, RSEI provides a valuable tool to measure general trends based upon relative risk-related impacts of TRI chemicals. Although RSEI results do not capture all environmental releases of concern, they generally relate changes in releases to relative changes in chronic human health impacts from a large number of toxic chemicals of concern to the Agency. Importantly, RSEI provides an ability to analyze the relative contribution of chemicals and industrial sectors to human health impacts, and RSEI

results serve as an analytical basis for setting priorities for further risk analysis, pollution prevention, regulatory initiatives, enforcement targeting, and chemical testing requirements.

## ES-2. General Description of the RSEI Chronic Human Health Model

The RSEI Chronic Human Health model calculates values that reflect the risk-related impacts on chronic human health of modeled TRI chemical releases and transfers. These values do not provide absolute measures of risk and can only be interpreted as relative measures to be compared with other such values (reflecting the direction and the general magnitude of changes at different points in time when analyzing trends, or identifying the relative contribution of variables in a comparative analysis).

The model uses the reported quantities of TRI releases and transfers of chemicals to estimate the risk-related impacts associated with each type of air and water release or transfer by every TRI facility. The risk-related impacts potentially posed by a chemical are a function of chemical toxicity, the fate and transport of the chemical in the environment after it is released, the pathway of human exposure, and the number of people exposed.<sup>1</sup>

The RSEI model starts with TRI releases. For each exposure pathway associated with each chemical release, the model generates an "Indicator Element." For instance, a release of the chemical benzene to air via a stack from the "ABC" Facility in 1999 is an "Indicator Element." Each Indicator Element is associated with a set of results, including pounds-based, hazard-based, and risk-related results, or scores. The risk-related score is a unitless value proportional to the potential risk-related impact of each element.

Each Indicator Element can be combined and compared with other Indicator Elements. There are countless ways that Indicator Elements can be grouped together to assess chronic human health impacts. For example, all of the RSEI results can be aggregated for each year to allow an assessment of trends in estimated impacts, or results can be grouped to allow users to compare results for facilities, regions, chemicals, and any combinations of these and other variables. RSEI does not perform a detailed or quantitative risk assessment, but offers a screening-level, risk-related perspective for relative comparisons of chemical releases. The model does not estimate actual risk to individuals. RSEI results are only meaningful when compared to other results produced by RSEI.

<sup>&</sup>lt;sup>1</sup> The method is focused on general populations; individuals, particularly highly exposed individuals, are not the focus of the model.

The current version of the model calculates risk-related results for the air and surface water pathways only. For other pathways, and in instances where information needed to model a release is not available, only pounds-based and hazard-based perspectives are available. In cases where toxicity weights are not available, only pounds-based results can be viewed.

#### ES-2.1 Geographic Basis of the Model

The model relies on the ability to locate facilities and people geographically, and to attribute characteristics of the physical environment, such as meteorology, to areas surrounding the facilities once they are located. To locate the facilities and the attribute data to those facilities, the model describes the U.S. and its territories<sup>2</sup> as a 1 km by 1 km grid system. For each cell in the grid, a location "address" in terms of (X,Y) coordinates is assigned based on latitude and longitude (lat/long). The origin of the grid is set at the intersection of the prime meridian and the equator, so the X coordinate is the distance in kilometers from the prime meridian to the latitudinal coordinate of the cell, and the Y coordinate is the distance in kilometers from the equator to the longitudinal coordinate of the cell. Each cell approximates a 1 sq km area.

In order to estimate potential exposure, TRI facilities and the U.S. population must be geographically located on the model grid. TRI facilities are located using the facilities' lat/long coordinates. To locate population, the model uses U.S. Decennial Census data for 1990 and 2000 at the block level. These data<sup>3</sup> are used to create detailed age-sex-defined population groups for each of the census blocks in the US for 1990 and for 2000. The following population groups are used in the model:<sup>4</sup>

- Males Aged 0 through 9 years
- Males Aged 10 through 17 years
- Males Aged 18 through 44 years
- Males Aged 45 through 64 years
- Males Aged 65 Years and Older

<sup>&</sup>lt;sup>2</sup> The model also includes Puerto Rico, the U.S. Virgin Islands, Guam, American Samoa, and the Northern Mariana Islands. U.S. Census data were provided by GeoLytics, Inc., East Brunswick, NJ.

<sup>&</sup>lt;sup>3</sup> For 1990, not all of the variables were available at the block level for the Continental U.S, Alaska and Hawaii. For those variables that were only available at the block group level, block group ratios were calculated and applied to the data at the block level. For 2000, all of the required data were available at the block level. For the U.S. Virgin Islands and the territories, data from larger geographic units (block groups or county-equivalents) were used. For Puerto Rico, block group data was used for 1990 and block-level data for 2000.

<sup>&</sup>lt;sup>4</sup> Not all of the population groups listed are used in viewing results. Model results can only be viewed for the following groups: Children Under 10, Children 10 through 17, Males 18 through 44, Females 18 through 44, and Adults 65 years and Older.

- Females Aged 0 through 9 years
- Females Aged 10 through 17 years
- Females Aged 18 through 44 years
- Females Aged 45 through 64 years
- Females Aged 65 Years and Older

Because the Census block boundaries have changed between 1990 and 2000, each set of Census block level data is first transposed onto the model grid, which is unchanging, using an area-weighted method. Once populations for 1990 and 2000 are placed on the grid, the model uses a linear interpolation in each grid cell to create annual estimates of the population sizes for each year between 1990 and 2000. The straight line plot is extrapolated to estimate population for 1988 and 1989.

Once facilities and people are located on the model's grid, three main components are used to compute risk-related impacts in the model. These components are:

- the quantity of chemicals released or transferred,
- adjustments for chronic human health toxicity, and
- adjustments for exposure potential and population size.

These components and the method used to combine them are described in the following sections.

**Chemical Releases and Transfers.** The model uses information on facilities' chemical releases and transfers from these facilities to off-site facilities (such as sewage treatment plants and incinerators) to model risk-related impacts. These releases are reported by facilities to the Toxics Release Inventory (TRI), as mandated by the Emergency Planning and Community Right-to-Know Act. As of the 2000 reporting year, there are 610 TRI chemicals and chemical categories listed. Users can view pounds of chemicals released per year (pounds-based results) for any combination of variables included in the model.

Adjustments for Chronic Human Health Toxicity. The model is based on current EPA methodologies for assessing toxicity. The method EPA has chosen for assigning toxicity weights to chemicals is clear and reproducible, based upon easily accessible and publicly available information, and uses expert EPA-wide judgments to the greatest extent possible. RSEI reflects the toxicities of chemicals relative to one another using a continuous system of numerical weights. Toxicity weights for chemicals increase as the toxicological potential to cause chronic human health effects increases. Toxicity-adjusted releases are called "hazard-based results" and provide an alternative perspective to pounds-based or full risk-related results, and are especially valuable when necessary data for risk-related modeling are not available.

Values developed by EPA experts are used to differentiate the degrees and types of toxicity of chemicals, and rank them in a consistent manner. Values called Oral Slope Factors and Inhalation Unit Risks<sup>5</sup> provide information pertaining to toxicity for chemicals that may cause cancer. Reference Doses (RfDs) and Reference Concentrations (RfCs) provide toxicity information related to noncancer effects.<sup>6</sup> Where these values are not available from EPA, other data sources may be used.

The following data sources are used, in the order of preference:

- EPA's Integrated Risk Information System (IRIS);
- EPA Office of Pesticide Programs' Acute and Chronic Reference Doses Table and List of Chemicals Evaluated for Carcinogenic Potential (OPP);
- Final, published Minimum Risk Levels (MRLs) from the Agency for Toxic Substances and Disease Registry (ATSDR);
- Final published toxicity values from California Environmental Protection Agency's Office of Environmental Health Hazard and Assessment (CalEPA);
- EPA's Health Effects Assessment Summary Tables (HEAST); and
- Final Derived/Interim Derived Toxicity Weights estimated by EPA's Office of Pollution Prevention and Toxics (Derived).

The toxicity scoring method separately evaluates exposure routes (inhalation and oral) and classes of effects (cancer and noncancer). For each exposure route, chemicals are scored based on their single most sensitive adverse effect; if a chemical exhibits both cancer and noncancer effects, the higher of the two weights is assigned as the final weight for that route. The following algorithms are used to assign toxicity weights:

non-carcinogens:	0.5 / RfD (mg/kg-day) or $1.8$ / RfC (mg/m <sup>3</sup> )
carcinogens (WOE categories A and B):	Oral Slope Factor (risk per mg/kg-day)/ 0.0005 or Inhalation Unit Risk (risk per mg/m <sup>3</sup> )/ 0.00014

<sup>&</sup>lt;sup>5</sup> The Oral Slope Factor represents the upper-bound (approximating a 95% confidence limit) estimate of the slope of the dose-response curve in the low-dose region for carcinogens. The units of the slope factor are usually expressed as (mg/kg-day) <sup>-1</sup>. The Inhalation Unit Risk is the upper-bound excess lifetime cancer risk estimated to result from continuous exposure to an agent at a concentration of 1  $\mu$ g/m<sup>3</sup> in air.

<sup>&</sup>lt;sup>6</sup> RfDs and RfCs are estimates (with uncertainty spanning perhaps an order of magnitude) of daily exposure [RfD], or continuous inhalation exposure [RfC], to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious noncancer effects during a lifetime.

carcinogens	Oral Slope Factor (risk per mg/kg-day)/ (0.0005 * 10)
(WOE category C):	or Inhalation Unit Risk (risk per mg/m <sup>3</sup> )/ (0.00014 * 10)

The distribution of toxicity values for TRI chemicals corresponds to a range of toxicity weights of approximately 0.01 to 1,000,000. However, toxicity weights are not bounded. Continuous toxicity weights are expressed as values with two significant figures.

There are 610 chemicals and chemical categories on the 2000 TRI Chemical List. Toxicity weights are available for 426 of these chemicals and chemical categories. Chemicals with toxicity weights account for over 98% of the reported pounds for all on-site releases in 2000.

Adjustments for Exposure Potential and Population Size. Quantitatively, exposure potential is estimated using a "surrogate" dose. To estimate the surrogate dose, a separate exposure evaluation is conducted for each pathway-specific chemical emission. The exposure evaluations use models that incorporate data on pathway-specific chemical releases and transfers, physicochemical properties and, where available, site characteristics, to estimate the ambient chemical concentration in the medium into which the chemical is released or transferred. The ambient concentrations are combined with human exposure assumptions and estimates of exposed population size specific to age and sex.

The algorithms for calculating surrogate doses rely on the ability to locate facilities and people geographically on the 1 km by 1 km grid cell system described earlier. While this method uses the EPA exposure assessment paradigm to evaluate exposure potential, the results should not be construed as an actual numerical estimate of dose resulting from TRI releases, because limited facility-specific data and the use of models that rely on default values for many parameters prevent the calculation of an actual dose. Instead, the purpose of the methodology is to generate as accurate a surrogate dose as possible without conducting an in-depth risk assessment. The estimates of surrogate doses from releases of TRI chemicals are *relative to the surrogate doses resulting from other releases included in the model*. Please note that not all pathways are currently modeled.

#### ES-2.2 RSEI Results

Because of the multi-functional nature of the model, a variety of results can be created. All RSEI results are based on the Indicator Element, which is a unique combination of facility,

chemical, release pathway, exposure pathway, and year<sup>7</sup>. Each Indicator Element has a set of associated results:

Risk-related results	Surrogate Dose <b>x</b> Toxicity Weight <b>x</b> Population
Hazard-based results	Pounds <b>x</b> Toxicity Weight
Pounds-based results	TRI Pounds released

Exhibit ES-1. Description of RSEI Approach

**Risk-related results.** The pathway-specific toxicity weight, surrogate dose, and population components are multiplied to obtain a risk score for the Indicator Element. The surrogate dose is determined through pathway-specific modeling of the fate and transport of the chemical through the environment, combined with subpopulation-specific exposure factors. The score is a unitless measure that is *not* independently meaningful, but is a risk-related estimate that can be compared to other estimates calculated using the same methods. If the Indicator Element cannot be modeled, because of a lack of data needed for modeling or because the release pathway is not currently modeled, then the risk-related score is zero. The model calculates risk-related results for the entire population and also for the following subpopulations: children under 10, children aged 10 to 17, males aged 18 to 44, females aged 18 to 44, and adults aged 65 and older. In addition, the model also calculates "Modeled Pounds," which is simply the number of pounds that can be modeled, before fate and transport modeling and exposure assumptions have been applied.

**Hazard-based results.** Each Indicator Element also is associated with a hazard-based result ("Hazard"), calculated by multiplying the pounds released by the appropriate chemical-specific toxicity weight (the toxicity weight also depends on the exposure pathway). The inhalation toxicity weight is used for releases or transfers to fugitive air, stack air, off-site incineration, and off-site incineration-no fuel value. The oral toxicity weight is used for releases or transfers to direct water and POTWs. For releases that are not modeled (because the pathway is not modeled or because other necessary data, such as physicochemical properties, are lacking), the higher

<sup>&</sup>lt;sup>7</sup> Several related Indicator Elements may be associated with certain release and exposure pathways (e.g., direct water releases may be associated with exposure from drinking water intakes, as well as fish ingestion from recreational fishing and from subsistence fishing).

toxicity weight is used. For these results, no exposure modeling or population estimates are involved. If there is no toxicity weight available for the chemical, then the hazard score is zero.

The model also calculates "Modeled Hazard," which is the chemical- and pathway-specific toxicity weights multiplied by the Modeled Pounds (as described above), and "Modeled Hazard \* Pop," which multiplies modeled hazard by the potentially exposed population, but without the fate and transport modeling (and application of exposure assumptions) that would be found in risk-related results.

**Pounds-based results.** These results ("TRI Pounds") reflect only the number of pounds released or transferred that are reported to TRI, and are available for virtually all Indicator Elements. The model also provides "TRI Pounds with Toxicity Weights," which simply sums the pounds for chemicals that have toxicity weights in RSEI.

Once results are calculated for each Indicator Element, they can be combined in many different ways. All of the results are additive, so a result for a specific set of variables is calculated by summing all the relevant individual Indicator Element results, as follows:

$$I = \sum \sum \sum IE_{c,f,p}$$
(Eq. ES.1)

where:

R = RSEI result, and  $IE_{c,f,p} =$  chemical-facility-pathway-specific Indicator Element result.

This method is very flexible, allowing for countless variation in the creation of results. For example, results can be calculated for various subsets of variables (e.g., chemical, facility, release pathway) and compared to each other to assess the relative contribution of each subset to the total potential impact. Or, results for the same subset of variables for different years can be calculated, to assess the general trend in pounds-based, hazard-based, or risk-related impacts over time.

It must be reiterated that while changes in results over the years would imply that there have been changes in hazard- or risk-related environmental impacts, the actual magnitude of any specific change or the reason may not be obvious. Although the value itself may be useful in identifying facilities or chemicals with the highest potential for hazard or risk, the score does not represent a quantitative estimate or provide an exact indication of the magnitude of individual hazard or risk associated with that facility or chemical.

#### ES-2.3 Adjusting RSEI Results for Changes in TRI Reporting

When a change occurs in the number of, or reporting requirements for, chemicals and facilities represented in TRI, the numerical value of RSEI results will be altered if no adjustments are made to the method of calculation to account for the changes respective to trend analyses. However, such changes would not necessarily represent a large change in actual environmental impact, but would reflect a broader understanding of the impacts that may have always existed. To maintain comparability in the weights over time, the results must be adjusted in some manner when such changes in TRI reporting occur.

A change in the number of chemicals and facilities in the TRI database can occur through several mechanisms. The addition to or deletion of chemicals from the TRI chemical list will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. The largest revision to the list occurred in November 1994, when the Agency added 245 chemicals and chemical categories to the existing TRI chemical list, effective for the reporting year 1995. Other revisions have occurred since. To allow for meaningful trend analysis, the model maintains a list of "core" chemicals which have been reported since 1987, and for which reporting requirements have not changed.

Compliance with TRI reporting has changed over time, which has led to more facilities reporting. Increases in the number of reporting facilities may also occur as a result of changes in reporting requirements. For instance, in the first two years of reporting, facilities that manufactured or processed more than 50,000 pounds were required to report their releases. However, EPCRA lowered this threshold to 25,000 pounds in 1989. And for reporting year 2000, thresholds and other reporting requirements for 18 Persistent Bioaccumulative Chemicals (PBTs) have been changed. Effective for reporting year 1998, TRI has enlarged the set of facilities required to report to include electric utilities, mining facilities, commercial hazardous waste facilities, solvent recovery facilities, and wholesale chemical and petroleum terminal facilities. All of these modifications can act to alter the total emissions reported on the TRI and the model's estimate of the associated relative risk-based impacts.

When deletions from the chemical list of TRI chemicals occur, RSEI's chemical database is modified to remove all results from previous reporting years. Also, the yearly TRI data for a given chemical list of chemicals and facilities are the subject of ongoing quality control review and correction by both EPA and reporting facilities. As a result, yearly comparisons could be flawed if such revisions in reported data were not included in each previous year's results. Therefore, the Indicator Elements are recomputed for all years on an annual basis in order to incorporate chemical deletions and revisions to the reporting data.

#### ES-2.4 Model Implementation

The RSEI Chronic Human Health model is currently implemented in a Microsoft Windowsbased computer program. The program allows users to calculate RSEI results for all years of data and to present the results in various GIS, graphical, and tabular formats, as well as to save selected data to spreadsheet and database formats (e.g., Microsoft Excel and databases such as Access). The program includes on-line help for all of the program functions, as well as an introductory, "Easy RSEI" interface that simplifies first-time use. A User's Manual is also available.

Users of the model can perform, in a matter of minutes or hours, a variety of screening-level analyses. Previously, such activities would have taken days, weeks, or even months to organize the relevant information, evaluate that information, and perform the complex and sophisticated analyses that are necessary to provide a risk-related perspective. Results can be used for screening-level ranking and prioritization for strategic planning purposes, risk-related targeting, and trends analyses. Considerable resources can be saved by conducting preliminary analyses with the model to identify risk-related situations of high potential concern, and which warrant further evaluation.

As noted above, users can evaluate releases using a number of variables, such as chemical, medium, geographic area or industry. For instance, the following types of questions can be investigated: How do industry sectors compare to one another from a risk-related perspective? What is the relative contribution of chemicals within a given industry sector? What release pathway for a particular chemical poses the greatest risk-related impacts? Users can view pounds-based, hazard-based, and other results, to investigate the relative influence of toxicity and population components on the risk-related results, which also incorporate exposure modeling.

The model also contains fully integrated geographic capabilities. Users can select facilities geographically and display maps. For a 101-kilometer square around a facility, the model will quickly and easily display grid-cell concentrations from chemical releases to air, and can sum the overlapping release plumes. In addition, for any small geographic area, users can display the population distribution for any population subgroup, and show the population- and toxicity-weighted air concentrations by subgroup in individual grid cells.

Information regarding the RSEI project is available on OPPT's RSEI web site.<sup>8</sup> Complete documentation, frequently asked questions, and contact information are all posted on the site. Periodic updates and troubleshooting information are also available for users.

# ES-2.5 How the RSEI Chronic Human Health Toxicity Weightings Differ from EPCRA Section 313 Statutory Criteria

As described above, the RSEI model uses Toxics Release Inventory (TRI) chemical reporting data. However, it is important that the public not confuse the use of the model as a screening-level tool for investigating relative risk-based impacts related to the releases and transfers of TRI chemicals, with the very different and separate activity of listing/delisting chemicals on the TRI using statutory criteria.

The goal of RSEI is to use data reported to the Agency to investigate the relative risk-based impacts of the releases and transfers of these chemicals on the general, non-worker population. The model differentiates the relative toxicity of listed chemicals and ranks them in a consistent manner. The ranking of each chemical reflects its toxicity only relative to other chemicals that are included in the model. Toxicity is not compared to some benchmark or absolute value as is required when adding or removing a chemical from the TRI. Furthermore, the model addresses only the single, most sensitive toxicity endpoint for chronic human health.

In contrast, the EPCRA statutory criteria used for listing and delisting chemicals consider acute and chronic human toxicity, as well as environmental toxicity, and considers multiple effects and the severity of those effects. The criteria also address the "absolute" chronic toxicity of chemicals on the TRI relative to a benchmark value.

Because of these differences, the toxicity weightings in the model cannot be used as a scoring system for evaluating listing/delisting decisions. RSEI does not attempt to reflect the statutory criteria for these chemicals.

<sup>&</sup>lt;sup>8</sup> For current information or inquiries regarding the Risk-Screening Environmental Indicators Project, please contact: Gary Cole, Ph.D., (202) 564-8811, cole.gary@epa.gov, or Cody Rice, (202) 564-8769, rice.cody@epa.gov. Or, see www.epa.gov/oppt/rsei/.

# ES-3. Important Caveats Regarding the RSEI Chronic Human Health Model

The RSEI Chronic Human Health model is a screening tool that provides a risk-related perspective in assessing the relative impacts of releases of toxic chemicals. Risk-related results are available for releases and transfers to air and water, and pounds- and hazard-based results are available for all media. RSEI combines estimates of toxicity, exposure level, and the exposed population to provide risk-related comparisons. It does not provide a detailed or quantitative assessment of risk, and is not designed as a substitute for more comprehensive, site-specific risk assessments. There are a number of important considerations associated with each component of the model, as described in the following sections.

**Toxicity Component.** The following caveats should be considered regarding the toxicity component of the model:

- Toxicity weights are not designed to (and may not) correlate with statutory criteria used for listing and delisting chemicals in TRI. RSEI risk-related model results account for estimated exposure and may not correlate with listing/de-listing decisions.
- The Chronic Human Health model only addresses chronic human toxicity (cancer and noncancer effects, e.g., developmental toxicity, reproductive toxicity, neurotoxicity, etc.) associated with long-term exposure and does not address concerns for either acute human toxicity or environmental toxicity.
- Toxicity weights are based upon the single, most sensitive chronic human health endpoint for inhalation or oral exposure pathways, and do not reflect severity of effects or multiple health effects.
- Estimated Reference Doses and Reference Concentrations for noncancer effects incorporate uncertainty factors which are reflected in toxicity weights that are based upon these values.
- Several significant assumptions are made regarding metals and metal compounds, because important data regarding these chemicals are not subject to TRI reporting. Metals and metal compounds are assumed to be released in the valence (or oxidation) state associated with the highest chronic toxicity weight (for chromium, the higher valence state has greater toxicity, e.g., Cr<sup>+6</sup> vs. Cr<sup>+3</sup>). Metal compounds are assumed to have the same toxicity weight as the parent metal, although the chronic toxicity of some metal compounds may be higher or lower.

While the physical form of released metals or metal compounds can affect toxicity, a reasonable assumption is made regarding the likely form of most releases (e.g., the non-cancer toxicity weight for chromic acid mists and dissolved hexavalent chromium aerosols is much higher than for hexavalent chromium particulates, but releases of these chemicals as acid aerosols are not expected to be typical so the toxicity weight for cancer based on the inhalation of particulates is used). Analysts need to consider these assumptions, and whether the gathering of additional data is warranted, when examining model results for metals and metal compounds.

**Exposure Component.** The following caveats should be considered regarding the exposure component of the model:

- Like other exposure models, RSEI estimates exposure levels (it does not yield actual exposures). The model provides estimated air concentrations in each grid cell.
- The model uses some generic assumptions, e.g., default median stack heights, diameters, and exit gas velocities related to 2- or 3-digit Standard Industrial Classification (SIC) codes, or a nationwide median, where facility-specific median stack height, diameter, and exit gas velocity data are unavailable.
- In the current version of the model, only air and direct surface water exposures are fully modeled.
- The model does not account for population activity patterns.
- The model has greater uncertainty when examining disaggregated results at the local or facility level.

**Population Component.** The following caveats should be considered regarding the population component of the model :

- Population values for non-decennial years are estimated based on linear interpolations at the block level between the 1990 and 2000 U.S. Census dates, and on extrapolations back to 1988.
- Drinking water populations are estimated by using the total drinking water populations associated with individual downstream drinking water intakes. Estimated populations for the fish ingestion pathway are based upon U.S. Fish and Wildlife Service surveys.

• Because RSEI results reflect changing population size at the local level, a facility's relative contribution could increase or decrease even without changes in its releases over time. While the model is designed to reflect the overall risk-related impacts on the local population, such population changes should be considered when examining a facility's environmental management practices.

# 1. Introduction

EPA's Risk-Screening Environmental Indicators (RSEI) is a screening-level tool that assesses the potential impact of industrial releases from pounds-based, hazard-based, and risk-related perspectives. RSEI uses risk concepts to quickly and easily screen large amounts of data, saving time and resources. RSEI is particularly useful for examining trends to measure change, ranking and prioritizing chemicals and industry sectors for strategic planning, conducting risk-related targeting, supporting community-based projects, and investigating environmental justice issues.

Using estimates of pounds of chemical releases to investigate potential health and environmental impacts is limited by the assumptions that all chemicals are equally toxic and all people are equally exposed. Formal risk assessments are more accurate, but are complicated and time consuming to prepare, requiring detailed data which is not always available, and the results are often limited in scope and geographic area. The RSEI approach augments estimates of pounds released with toxicity and exposure considerations, but does not address all of the potential factors that a full risk-assessment would include.

RSEI considers the following information: the amount of chemical released, the toxicity of the chemical, its fate and transport through the environment, the route and extent of human exposure, and the number of people affected. This information is used to create numerical values that can be added and compared in limitless ways to assess the relative risk of chemicals, facilities, regions, industries, or many other factors. The values are for comparative purposes and only meaningful when compared to other values produced by RSEI. It should be emphasized that the result is *not* a detailed or quantitative risk assessment, *but offers a screening-level, risk-related perspective for relative comparisons of chemical releases*.

The RSEI approach is very flexible and can be implemented in various ways. The use of the model is not limited to TRI chemicals; in principle, the adaptable method can model any chemical if toxicity characteristics, physicochemical properties, release levels, and release location are known or can be estimated. RSEI is currently implemented as the RSEI Chronic Human Health model, which addresses chronic human health effects and chronic exposures, and uses estimates of annual releases from EPA's Toxics Release Inventory (TRI).

# 1.1 Background

In 1989, EPA outlined the goals for establishing strategic planning processes at the Agency (EPA, 1990c). Underlying this approach was the Agency's desire to set priorities and direct resources to areas with the greatest opportunity to achieve health and environmental risk reductions. As part of this initiative, the Administrator set forth a plan to develop indicators to track changes in environmental health impacts over time. Tracking these changes would allow the Agency to measure its progress in implementing environmental protection and pollution prevention programs. In addition, comparing the relative contribution of particular chemicals,

Version 2.1 January 2004 industries and geographic regions through the indicators would allow the Agency (and other users) to establish priorities for improving human health and the environment.

To efficiently track changes in human health and environmental impacts over time, the Agency should take advantage of existing data sources that reflect multimedia trends in environmental contaminant releases. The Toxics Release Inventory (TRI) is one of the Agency's most relevant source of continuous data for developing indicators of change in environmental impacts over time. The TRI is mandated by the Emergency Planning and Community Right-to-Know Act (EPCRA) Title III Section 313 and requires that U.S. manufacturing facilities file annual reports documenting multimedia environmental releases and off-site transfers for more than 600 chemicals and chemical categories which are of concern to the Agency.

In response to the need for environmental indicators, and to take advantage of the rich data source offered by the TRI, the Office of Pollution Prevention and Toxics (OPPT) convened a workgroup to explore the development of an indicator or indicators based on the TRI that could track changes in human health and environmental impacts. Specifically, the approach would integrate toxicity, exposure and population considerations into the risk-related evaluation of releases. The RSEI model was developed in response to this initiative.

When evaluating impacts of chemicals, it is important to not only consider the number of pounds of a chemical released to the environment, but also the toxicity of the chemical, its exposure potential, and the size of the receptor population. RSEI integrates these factors and provides a relative risk-based perspective of chemical releases and transfers. To the extent possible, the RSEI Chronic Human Health model is based on existing EPA approaches, data, and models, to minimize duplication of effort and to maximize consistency with other Agency efforts to evaluate human health impacts.

The current version of the model tracks changes in chronic human health impacts. Ultimately, the model may be expanded to track acute human health and chronic and acute ecological impacts.

This document explains how the RSEI model is constructed, and describes the conceptual method, data sources, and the computational approach. The aim is to explain the model to a variety of agencies and groups that may wish to use or adapt the model, or the RSEI methodology in general, to their own needs. In addition, it describes the advantages of the RSEI approach in terms of flexibility, power, and usefulness as an analytical and strategic policy planning tool.

### 1.2 Model Implementation

The RSEI Chronic Human Health model is currently implemented in a Microsoft Windowsbased computer program. The program allows users to calculate RSEI results for all years of data beginning with 1988 reporting, and to present the results in various GIS, graphical, and tabular formats, as well as to save selected data to spreadsheet and database formats (e.g., Microsoft Excel and databases such as Access). The program includes on-line help for all of the program functions, as well as an introductory, "Easy RSEI" interface that simplifies first-time use. A User's Manual is also available.

Users of the RSEI model can perform, in a matter of minutes or hours, a variety of screeninglevel analyses. Previously, such activities would have taken days, weeks, or even months to organize the relevant information, evaluate that information, and perform the complex and sophisticated analyses that are necessary to provide a risk-related perspective. Results can be used for screening-level ranking and prioritization for strategic planning purposes, risk-related targeting, and trends analyses. Considerable resources can be saved by conducting preliminary analyses with the RSEI model to identify risk-related situations of high potential concern, and which warrant further evaluation.

Users can evaluate releases using a number of variables, such as chemical, medium, geographic area or industry. For instance, users can investigate the following types of questions: How do industry sectors compare to one another from a risk-related perspective? What is the relative contribution of chemicals within a given industry sector? What release pathway for a particular chemical poses the greatest risk-related impacts? Users can view pounds-based, hazard-based, and other results, to investigate the relative influence of toxicity and population on the risk-related results, which also incorporate exposure modeling.

The model also contains fully integrated geographic capabilities. Users can select and display facilities geographically. For a 101 kilometer square around a facility, the model will quickly and easily display grid-cell concentrations from chemical releases to air, and sum up the overlapping release plumes. In addition, for any small geographic area, the model can display the population distribution for any population subgroup, and show the population- and toxicity-weighted air concentrations by subgroup in individual grid cells.

Information regarding the RSEI project is available on OPPT's RSEI web site, at www.epa.gov/oppt/rsei/.

## **1.3 Organization of this Document**

Chapter 2 of this document gives a brief description of the RSEI method and the Chronic Human Health model, as well as a discussion of their overall strengths and limitations. Chapter 3 describes the TRI emissions data used in the model. Chapter 4 describes the methods used to adjust the emissions data for chemical toxicity, and Chapter 5 provides a discussion of the geographic basis of the model, as well as pathway-specific descriptions of adjustments made for exposure potential and population size. Chapter 6 presents the equations for calculating RSEI results, and Chapter 7 describes issues pertinent to the current implementation of the RSEI method.

There are also six Technical Appendices that accompany this methodology document and provide additional information on the data used in the model. The Appendices are as follows:

Technical Appendix A- Listing of All Toxicity Weights for TRI Chemicals and Chemical Categories

Technical Appendix B- Physicochemical Properties for TRI Chemicals and Chemical Categories Technical Appendix C- Derivation of Model Exposure Parameters

Technical Appendix D- Locational Data for TRI Reporting Facilities and Off-site Facilities

Technical Appendix E- Derivation of Stack Parameter Data

Technical Appendix F- Summary of Differences Between RSEI Data and the TRI Public Data Release

In addition, two documents containing background and supporting information are available on the project web site. *Analyses Performed for the Risk-Screening Environmental Indicators* contains three parts: Part A describes the result of a ground-truthing analyses performed to determine the accuracy of the air pathway modeling; Part B contains additional analyses performed on the air pathway to determine optimal modeling parameters; and Part C describes the results of an analysis of SIC code-based stack parameter data. *Developing the Risk-Screening Environmental Indicators* describes the development of the model, and outlines options that were considered for several important aspects of the method. These background documents are available on the RSEI web site at www.epa.gov/oppt/rsei. The RSEI web site also contains complete methodological information, a document archive, the RSEI User's Manual, RSEI Tutorials, answers to frequently asked questions, contact information, and a glossary.

# 2. General Description of the RSEI Chronic Human Health Model

## 2.1 General Description

The RSEI Chronic Human Health model is a screening-level tool that assesses the potential impact of TRI releases from pounds-based, hazard-based, and risk-related perspectives. A basic outline of the modeling approach is illustrated in Exhibit 2.1.

Three main components are used in the model to calculate results:<sup>1</sup>

- The Toxics Release Inventory (TRI), maintained by EPA, provides the data on the **quantity of chemicals** released to air, water, on-site disposal facilities, and transferred to off-site facilities for the more than 600 toxic chemicals that are listed on the TRI. Reporting by facilities to the TRI began in 1987, and has continued each year since then (RSEI uses TRI reporting data beginning in 1988). Releases are reported in pounds per year.
- **Toxicity weights** are assigned to each chemical for which adequate data are available. These weights are assigned using quantitative toxicity values developed by EPA scientists and additional qualitative assessments, as described below.
- **Exposure and population modeling** are performed for the air and surface water pathways to model the movement of each chemical release through the environment to the exposed population. A surrogate dose, the amount of chemical that a human contacts, is estimated. The estimation of a surrogate dose allows comparisons across pathways. Then the population exposed to each release is estimated using U.S. Decennial Census data.

<sup>&</sup>lt;sup>1</sup> The method focuses on general populations: individuals, particularly highly exposed individuals, are not the focus of the Chronic Human Health model. Furthermore, worker exposures are not addressed.

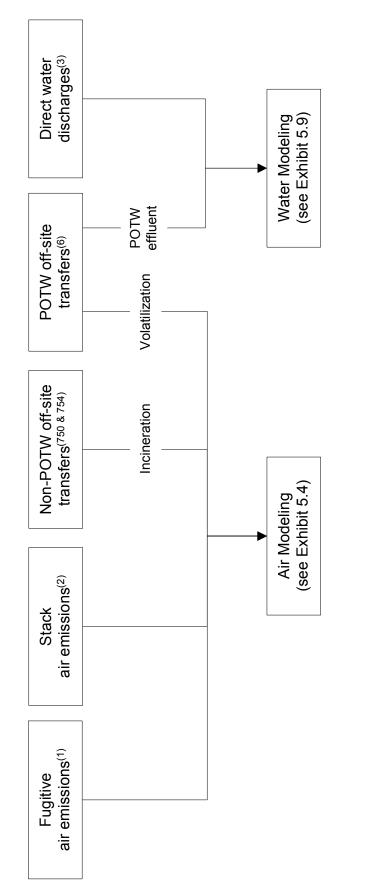


Exhibit 2.1 RSEI Chronic Human Health Modeling Approach

<sup>(1)</sup> indicates media code 1: Fugitive Air Release

<sup>(2)</sup> indicates media code 2: Stack Air Release

(750) indicates media code 750: Offsite Incineration/ Thermal Treatment Release

(754) indicates media code 754: Offsite Incineration (no fuel value) Release

(6) indicates media code 6: POTW Transfer

<sup>(3)</sup> indicates media code 3: Direct Water Release

The RSEI model starts with TRI releases. For each exposure pathway associated with each chemical release, the model generates an "Indicator Element." For instance, a release of the chemical benzene to air via a stack from the "ABC" Facility in 1999 is an "Indicator Element."<sup>2</sup> Each Indicator Element is associated with a set of results, including pounds-based, hazard-based, and risk-related results, or scores. The risk-related score is a unitless value proportional to the potential risk-related impact of each element.

Exhibit 2.2 Description of RSEI Results

Risk-related results	Surrogate Dose <b>x</b> Toxicity Weight <b>x</b> Population
Hazard-based results	Pounds <b>x</b> Toxicity Weight
Pounds-based results	TRI Pounds released

**Risk-related results.** The toxicity, surrogate dose, and population components are multiplied to obtain a risk score for the Indicator Element. The surrogate dose is determined through pathway-specific modeling of the fate and transport of the chemical through the environment, combined with subpopulation-specific exposure factors. The score is a unitless measure that is *not* independently meaningful, but is a risk-related estimate that can be compared to other estimates calculated using the same methods. If the Indicator Element cannot be modeled, because of the lack of data needed for modeling or because the release pathway is not currently modeled, then the risk-related score is zero. The model calculates risk-related results for the entire population and also for the following subpopulations: children under 10, children aged 10 to 17, males aged 18 to 44, females aged 18 to 44, and adults aged 65 and older. In addition the model also calculates "Modeled Pounds," which is simply the number of pounds that can be modeled, before fate and transport modeling and exposure assumptions have been applied.

**Hazard-based results.** Each Indicator Element also is associated with a hazard-based result ("Hazard"), calculated by multiplying the pounds released by the appropriate chemical-specific toxicity weight (the toxicity weight also depends on the exposure pathway). The inhalation

<sup>&</sup>lt;sup>2</sup> Several related Indicator Elements may be associated with certain release and exposure pathways (e.g., direct water releases may be associated with exposure from drinking water intakes, as well as fish ingestion from recreational fishing and from subsistence fishing).

toxicity weight is used for releases or transfers to fugitive air, stack air, off-site incineration, and off-site incineration - no fuel value. The oral toxicity weight is used for releases or transfers to direct water and POTWs. For releases that are not modeled (because the pathway is not modeled or because other necessary data, such as physicochemical properties, are lacking), the higher toxicity weight is used. For these results, no exposure modeling or population estimates are involved. If there is no toxicity weight available for the chemical, then the hazard score is zero.

The model also calculates "Modeled Hazard," which is the chemical- and pathway-specific toxicity weights multiplied by the Modeled Pounds (as described above), and "Modeled Hazard \* Pop," which multiplies modeled hazard by the potentially exposed population, but without the fate and transport modeling (and application of exposure assumptions) that would be found in risk-related results.

**Pounds-based results.** These results ("TRI Pounds") reflect only the number of pounds released or transferred that are reported to TRI, and are available for virtually all Indicator Elements. The model also provides "TRI Pounds with Toxicity Weights," which simply sums the pounds for chemicals that have toxicity weights in RSEI.

Once results are calculated for each Indicator Element, they can be combined in many different ways. All of the results are additive, so a result for a specific set of variables is calculated by summing all the relevant individual Indicator Element results, as follows:

$$R = \sum \sum \sum IE_{c,f,p}$$
(Eq. 2.1)

where:

R = RSEI result, and  $IE_{c,f,p} =$  chemical-facility-pathway-specific Indicator Element result.

This method is very flexible, allowing for countless variation in the creation of results. For example, results can be calculated for various subsets of variables (e.g., chemical, facility, release pathway) and compared to each other to assess the relative contribution of each subset to the total potential impact. Or, results for the same subset of variables for different years can be calculated, to assess the general trend in pounds-based, hazard-based, or risk-related impacts over time.

It must be reiterated that while changes in results over the years would imply that there have been changes in hazard- or risk-related environmental impacts, the actual magnitude of any specific change or the reason may not be obvious. Although the value itself may be useful in identifying facilities or chemicals with the highest potential for hazard or risk, the score does not represent a quantitative estimate or provide an exact indication of the magnitude of individual hazard or risk associated with that facility or chemical.

### 2.2 Summary of the Strengths and Limitations of the RSEI Chronic Human Health Indicators Model

#### 2.2.1 Strengths

The following are strengths of the model:

- The model provides important hazard-based and risk-related perspectives regarding the impacts of TRI releases on chronic human health.
- The model quickly organizes and evaluates data in a complex manner. For example, the air exposure model is combined with U.S. Census data to directly estimate the size of exposed populations and subpopulations and the magnitude of their exposure, rather than assuming that all individuals surrounding a facility are equally exposed.
- The model allows for greatly increased speed in performing screening analyses, thereby conserving resources for conducting more precise, site-specific risk evaluations. In addition, its use as a priority-setting tool allows resources to be focused in areas that will provide the greatest risk reduction.
- The model can perform single- and multi-media analyses.
- Custom-designed selections can be based upon a wide range of variables.
- This adaptable method can model any chemical if toxicity characteristics, appropriate physicochemical properties, release levels and release location are known or can be estimated.
- The model considers both cancer and non-cancer human health endpoints.
- The RSEI method has been subject to repeated expert peer review.
- The model's methodology and assumptions are transparent. Complete and detailed documentation of the RSEI model is available.

#### 2.2.2 Limitations

The following are limitations of the model:

- RSEI results do not provide users with quantitative risk estimates (e.g., excess cases of cancer).
- RSEI results do not evaluate individual risk.
- The model does not account for all sources of TRI chemicals; it only accounts for those sources that are required to report to TRI. It also does not provide scores for all TRI chemicals, although chemicals without toxicity weights account for a very small percentage of total releases and of total risk-related impacts.
- TRI does not account for all toxic chemicals.
- The model assumes that air concentrations of TRI chemicals are the same for indoor and outdoor exposures, and that populations are continuously exposed.
- Dermal and food ingestion pathways (other than fish consumption), and some other indirect exposure pathways are not evaluated.
- Acute health effects associated with short-term, periodic exposures to higher levels of these same chemicals are not addressed.
- Ecological effects are not addressed.

# 3. TRI Emissions Data

The RSEI model uses information on chemical releases and transfers collected by the Toxics Release Inventory (TRI). The TRI is a publicly available EPA database that contains information on toxic chemical releases and other waste management activities reported annually by federal facilities and facilities in certain industry groups. TRI operates under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA). EPCRA's primary purpose is to inform communities and citizens of chemical hazards in their areas. Sections 311 and 312 of EPCRA require businesses to report the locations and quantities of chemicals stored on-site in order to help communities prepare to respond to chemical spills and similar emergencies. EPCRA Section 313 requires EPA and the States to annually collect data on releases and transfers of certain toxic chemicals from industrial facilities, and to make the data available to the public in the Toxics Release Inventory. In 1990 Congress passed the Pollution Prevention Act which required that additional data on waste management and source reduction activities be reported under TRI. The goal of TRI is to empower citizens, through information, to hold companies and local governments accountable in terms of how toxic chemicals are managed. EPA compiles the TRI data each year and makes it available through several data access tools, including the TRI Explorer and Envirofacts.<sup>3</sup>

The TRI release and transfer data reported each year are the initial source of quantitative data on potential chronic human exposure used in RSEI. However, the EPA has an open revision policy that allows facilities reporting to the TRI to submit changes and corrections to their TRI data at any time. To avoid the effects of these fluctuations on RSEI results, the model extracts release and transfer data during the two week period each year when EPA "freezes" the data, that is, when no changes are allowed. To ensure that each RSEI model update is current on all revisions to the TRI data, data for all years are extracted once a year during the "data freeze" period, and added to the model, replacing the previous data. The same data freeze is used in preparing EPA's TRI Public Data Release (PDR). It should be noted that the "frozen" data set is not necessarily the same as the TRI database publicly accessible through the Internet: EPA's TRI Explorer or Envirofacts are "live" databases that are regularly updated. Despite EPA's open revision policy, errors do still happen, and some errors remain in the system for more than one year. It is therefore important to perform additional inquiries and analyses to support and verify results from RSEI, which should only be used as a screening tool.

Even though the TRI PDR and RSEI both use the annual data freeze, there still are some important differences between the two data sets. RSEI performs considerable processing on the set of on-site and off-site facilities, including geocodoing their addresses, and identifying

<sup>&</sup>lt;sup>3</sup> This program description is from the TRI web site, http://www.epa.gov/tri/. The web site provides additional information, including reporting requirements for facilities.

duplicate records of off-site facilities. The TRI PDR adjusts its data to account for double counting of releases from RCRA-regulated chemical treatment, storage, and disposal (TSD) facilities. Additionally, each year there may be several corrections to individual facility releases that may be made in one database but not the other. For more detail on these differences and any year-specific differences, please see Technical Appendix F, "Summary of Differences Between RSEI Data and the TRI Public Data Release."

# 4. Methods for Calculating Toxicity Weights

The EPCRA Section 313 criteria list several human toxicity parameters that EPA must consider when evaluating a chemical for addition to TRI, including acute toxicity, cancer or teratogenic effects, serious or irreversible reproductive dysfunctions, neurological disorders, heritable genetic mutations, or other chronic health effects. EPCRA also considers environmental toxicity. Some chemicals have toxicity data for only one effect, while others have evidence of effects within several of these toxicity categories. The definition of types of toxicity as given in Section 313 are presented in Exhibit 4.1.

The RSEI model focuses on carcinogens and other types of chronic toxic effects that are typically associated with chronic exposures.<sup>4</sup> The method relies heavily on current EPA methodologies for assessing toxicity, and will be continually updated to reflect any changes in these methods.

Endpoint	Definition
Carcinogenicity	The ability of a chemical to produce cancer in animals or humans.
Heritable Genetic and Chromosomal Mutation	The failure to transmit genetic information. This can involve at least three separate modes of action: the 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	Interference with the development of normal reproductive capacity. Chemicals can affect gonadal function, the estrous cycle, mating behavior, conception, parturition, lactation, and weaning.
Acute Toxicity	The potential for a short-term exposure (typically hours or days) by inhalation, oral, or dermal routes to cause acute health effect or death.

#### Exhibit 4.1 Toxicity Endpoints

<sup>&</sup>lt;sup>4</sup> Chronic effects are those that generally persist over a long period of time whether or not they occur immediately after exposure or are delayed. Chronic exposure refers to multiple exposures occurring over an extended period of time, or a significant fraction of an individual's lifetime.

Endpoint	Definition
Chronic Toxicity	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	Changes to the central and/or peripheral nervous system, which may be morphological (biochemical changes in the system or neurological diseases) or functional (behavioral, electrophysiological, or neurochemical effects).

# 4.1 Toxicity Weighting Scheme for Non-carcinogens and Carcinogens

The RSEI method uses a proportional system of numerical weights that reflect the toxicities of chemicals relative to one another. The toxicity weights of chemicals increase as the toxicological potential to cause chronic human health effects increases. The method EPA has chosen for assigning toxicity weights to chemicals is clear and reproducible, based upon easily accessible and publicly available information, and uses expert EPA-wide judgments to the greatest extent possible.

Factors that could be used to weight a chemical's toxicity include: the number of these effects that it causes; the relative severity of the effects it causes; the potency of the chemical for one or more of these effects; and the uncertainty inherent in characterizing effects. The RSEI method focuses on the latter two factors (potency and uncertainty inherent in characterizing effects), and thus considers both quantitative and qualitative elements to judge the relative toxicity of chemicals. The types of data required and the method used to combine these data into toxicity weights are described below.

### 4.1.1 Qualitative Data

Uncertainty reflecting the quality and adequacy of the data is incorporated into the toxicity weights or in their underlying toxicity values. The approach is intended to differentiate the relative toxicity of these chemicals in a uniform manner.

When evaluating the potential toxicity of a chemical to humans, risk assessors use a variety of data, 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 judge qualitatively 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 weight-of-evidence classification. Weight-of-evidence (WOE) schemes can be designed to indicate whether a chemical either causes a specific health effect in general, or specifically in humans.

For **cancer** effects, the WOE system presented in this method relies on categorical definitions from the EPA Guidelines for Carcinogenic Risk Assessment (EPA, 1986a), which are related to the potential for a chemical to be carcinogenic to humans.<sup>5</sup> The Cancer Guidelines define the six WOE categories shown in Exhibit 4.2. In the RSEI model, weight-of-evidence categories A, B1, and B2 (known and probable carcinogens) are combined. The combination of the A and B categories represents a modification of the Hazard Ranking System (HRS), which is used by the EPA's Office of Emergency Response and Remediation to rank hazardous waste sites for inclusion in the National Priorities List. Under the HRS scheme, A, B, and C categories are each considered separately. This revision reduces the dichotomy between the A and B categories, a dichotomy that may be inappropriate in the context of assigning toxicity weights. Also, combining A and B categories stabilizes the model results against changes induced by chemicals switching between the A and B designations. Class C chemicals (possible carcinogens) are assigned weights by dividing the calculated toxicity weights by a factor of 10 (see Section 4.1.3), because evidence that they cause cancer in humans is less certain. The choice of applying a factor is based on the advice of peer review and the HRS; an order of magnitude difference is an arbitrary uncertainty factor. Categories D and E are not considered in this weighting scheme (i.e., no toxicity weight is assigned).

<sup>&</sup>lt;sup>5</sup> It should be noted that EPA's Cancer Guidelines are intended to be updated. Two additional weight-of-evidence schemes have been proposed: one in 1996 and one in 1999. Neither of these are final. The 1999 Draft EPA WOE categories (see www.epa.gov/ncea/raf/car2sab/preamble.pdf) are not grouped by letter as are the EPA's 1986 WOE categories. When only 1999 WOE's were available, they were translated into 1986 designations in the following way:

Carcinogenic to humans – A

<sup>•</sup> Likely to be carcinogenic to humans – B

<sup>•</sup> Suggestive evidence of carcinogenicity, but not sufficient to assess human carcinogenic potential – C

<sup>•</sup> Data are inadequate for an assessment of human carcinogenic potential – D

<sup>•</sup> Not likely to be carcinogenic in humans – E

Exhibit 4.2
Weight-of-Evidence Categories for Carcinogenicity

Category	Weight-of-Evidence
А	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.
C	Limited evidence of carcinogenicity in animals and an absence of evidence or data 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.

Source: 51 FR 33996

For **noncancer** effects, weight-of-evidence is considered qualitatively in the hazard identification step of determining an RfD or an RfC. The WOE evaluation for noncancer effects is different from that for carcinogenic effects. The WOE judgment for noncancer effects focuses on the dose where chemical exposure would be relevant to humans (Dourson, 1993). That is, the focus of the WOE evaluation and the expression of the level of confidence in the RfD is a judgment of the accuracy with which the dose relevant to humans has been estimated. The WOE evaluation is included qualitatively in the RfD, but does not affect its numerical calculation. Since weight-of-evidence has been considered in developing RfDs, RSEI does not consider WOE separately for noncancer effects.

#### 4.1.2 Quantitative Data

Quantitative data on the relative potencies of chemicals are needed for toxicity weighting. These data generally result from analyses done during the third stage of risk assessment, the dose-response assessment. This stage involves describing the quantitative relationship between the amount of exposure to a chemical and the extent of toxic injury or disease observed. Risk posed by exposure to a chemical cannot be described without quantitative dose-response data. Dose-response data are derived from animal studies or, less frequently, from studies in exposed human populations. There may be many different dose-response relationships for a chemical if it produces different toxic effects under different conditions of exposure.

For **cancer risk assessment**, EPA has developed standard methods for predicting the incremental lifetime risk of cancer per dose of a chemical. EPA quantitatively models the dose-response function of a potential carcinogen and typically provides estimates of Oral Slope Factors or Inhalation Unit Risks. The Oral Slope Factor represents the upper-bound estimate of the slope of the dose-response curve in the low-dose region for carcinogens, and is a measure of cancer potency. The units of the slope factor are usually expressed as  $(mg/kg-day)^{-1}$ . The Inhalation Unit Risk is the upper-bound excess lifetime cancer risk estimated to result from continuous exposure to an agent at a concentration of 1 µg/m<sup>3</sup> in air (RSEI toxicity weights are based on this value when expressed as risk per mg/m<sup>3</sup>). Although the level of conservatism inherent in the Oral Slope Factors and Unit Risks varies by chemical, Oral Slope Factors and Unit Risk Factors nonetheless are the best readily available values that allow a comparison of the relative cancer potency of chemicals.

For **noncancer risk assessment**, data on dose-response are typically (though not always) more limited; generally, a risk assessor evaluates dose compared to a Reference Dose (RfD) or Inhalation Reference Concentration (RfC). Both the RfD and RfC are defined as "an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure [or continuous inhalation exposure the RfC] to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious [noncancer] effects during a lifetime" (EPA, 1988a; EPA, 1990b). The units of RfD are mg/kg-day, while the units of the RfC are mg/m<sup>3</sup>. A chemical's Reference Dose or Reference Concentration is typically based on a No Observable Adverse Effect Level (NOAEL) or Lowest Observable Adverse Effect Level (LOAEL), combined with appropriate uncertainty factors to account for intraspecies variability in sensitivity, interspecies extrapolation, extrapolation from LOAELs to NOAELs, and extrapolation from subchronic to chronic data. 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. By definition, exposures below the RfD/RfC are unlikely to produce an adverse effect; above this value, an exposed individual may be at risk for the effect. Empirical evidence generally shows that as the dosage of a toxicant increases, the severity and/or incidence of effect increases (EPA, 1988a), but for a given dose above the RfD/RfC, the specific probability or severity of an effect is not known. For purposes of the RSEI model, it is assumed that noncancer risk varies as the ratio of the estimated dose to the RfD/RfC.

#### 4.1.3 Algorithm for Calculating Toxicity Weight

The RSEI method uses several different algorithms to assign toxicity weights.

non-carcinogens:	0.5 / RfD (mg/kg-day) or 1.8 / RfC (mg/m <sup>3</sup> )
<b>carcinogens</b> (WOE categories A and B):	Oral Slope Factor (risk per mg/kg-day)/ 0.0005 or Inhalation Unit Risk (risk per mg/m <sup>3</sup> )/ 0.00014
<b>carcinogens</b> (WOE category C):	Oral Slope Factor (risk per mg/kg-day)/ (0.0005 * 10) or Inhalation Unit Risk (risk per mg/m <sup>3</sup> )/ (0.00014 * 10)

Exhibit 4.3 Algorithms for Assigning Toxicity Weights

This scoring system is a modification of the Hazard Ranking System used by the EPA's Office of Emergency Response and Remediation. The HRS scoring matrices provide weights corresponding to toxicity values expressed in terms of dose, that is, mg of chemical per kg of body weight per day. However, toxicity values for the inhalation pathway are typically expressed in units of exposure, that is, mg of chemical per m<sup>3</sup> of air. The toxicity weighting methodology, therefore, uses standard adult human exposure factors for inhalation rate (20 m<sup>3</sup>/day) and body weight (70 kg) to modify toxicity values expressed in units of exposure. This adjustment means that different constants are used to calculate the toxicity weights when inhalation toxicity values are used rather than oral toxicity values (1.8 versus 0.5 for non-carcinogens, and 0.00014 versus 0.0005 for carcinogens). All RSEI toxicity weights are expressed as reciprocal units of mg/kg-day.

As these calculations show, noncancer toxicity weights are proportional to the reciprocal of the RfD or RfC for the oral and inhalation exposure pathways, respectively. Cancer toxicity weights are proportional to the slope factor or inhalation unit risk, for the oral and inhalation exposure pathways, respectively. When multiplied by the surrogate dose estimated by RSEI, the risk-related scores calculated by the model are unitless, and should be used only for comparative purposes within RSEI.

It should be noted that the toxicity weight calculation maintains the implicit equivalence between cancer and noncancer weights that was established in the Hazard Ranking System. That is, the HRS toxicity scoring system implies that exposure at the level of the RfD is equivalent to a  $2.5 \times 10^{-4}$  cancer risk, because both of these risks are assigned the same toxicity weight.

# 4.2 Selecting the Final Chronic Human Health Toxicity Weight for a Chemical

Inhalation and oral toxicity weights are developed separately. If values are available for each route, then separate toxicity weights are assigned to each route. If data are available for only one route, the same toxicity weight is applied for both routes, provided there is no evidence the effects are route-specific or limited to the "portal of entry" into the body. In rare instances, toxicity studies are available to show that a given chemical causes no effects via one route; in these instances, a toxicity weight is assigned only to the route that results in chronic human health effects. Although assigning the same weight to both routes is not an ideal method, it is appropriate for a screening-level tool like the RSEI model.

Although chemicals can cause several types of toxic effects, the model assigns a toxicity weight to a chemical based on the single most sensitive adverse effect for the given exposure route (oral or inhalation). If a chemical exhibits both carcinogenic and noncarcinogenic effects, the higher of the associated cancer and noncancer weights is assigned as the final weight for the chemical for the given route.

The approach of weighting based on the most sensitive adverse effect does not consider differences in the type, number or target of the effects posed by the chemicals. For example, liver toxicity is weighted in the same way that neurotoxicity is weighted; in principle, chemicals causing a certain type of effect could be assigned additional weight if special concern existed for that type of effect. However, applying such additional weights would require a subjective evaluation of the relative severity of the health effects. Also, chemicals with a broad range of adverse health effects are weighted the same as a chemical causing only one effect. This approach may appear to under-estimate the risk of chemicals with a broad spectrum of effects relative to chemicals with one or few effects. However, a chemical may appear to demonstrate just one adverse effect only because there are no data on other effects; thus, applying an additional weight based on the number of endpoints may undervalue some poorly-studied but still hazardous chemicals. For these reasons, the options for applying additional weights based on number and relative severity of endpoints were not adopted.

## 4.3 Sources of Data

Information regarding the human health effects data on the TRI chemicals is compiled from the following sources:

**IRIS.** The primary (and most preferred) source of these data is EPA's Integrated Risk Information System (IRIS). IRIS is available on the internet (at http://www.epa.gov/iris/), and includes information on EPA evaluations of chemical toxicity for both cancer and noncancer effects of chemicals. 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 Oral Slope Factors or Inhalation Unit Risk values for chemicals with carcinogenic effects as well as RfDs or RfCs for chemicals with noncancer effects. Data contained in IRIS have been peer-reviewed and represent Agency-wide expert judgments. The peer-review process involves literature review and evaluation of a chemical by individual EPA program offices and intra-Agency work groups before inclusion in IRIS.

**OPP.** EPA's Office of Pesticide Programs (OPP) Acute Chronic and Reference Doses Table lists OPP's evaluations of the noncarcinogenic potential of chemicals that are of interest to OPP. OPP also publishes the List of Chemicals Evaluated for Carcinogenic Potential, which examines carcinogens. Both of these lists are updated periodically.

**ATSDR.** The Agency for Toxic Substances and Disease Registry (ATSDR) is an agency of the U.S. Department of Health and Human Services, which deals with the effect on public health of hazardous substances in the environment. ATSDR develops Minimum Risk Levels (MRLs) for chemicals on the CERCLA National Priorities List. An MRL is an estimate of the daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse noncancer health effects over a specified duration of exposure. RSEI uses data from MRLs developed for chronic exposure only. MRLs are intended to serve as screening levels only, and are useful in identifying contaminants and potential health effects that may be of concern at hazardous waste sites. See http://www.atsdr.cdc.gov/mrls.html for more information on MRLs and specific values.

**CalEPA.** The California Environmental Protection Agency (CalEPA) Office of Environmental Health Hazard and Assessment (OEHHA) is responsible for developing and distributing toxicological and medical information needed to protect public health. RSEI uses final toxicity values published by CalEPA in the Consolidated Table of OEHHA & California's Air Resources Board (ARB) Approved Risk Assessment Health Values. The table is continuously updated and can be found on the internet at http://www.arb.ca.gov/toxics/healthval/healthval.htm.

**HEAST.** EPA's Health Effects Assessment Tables (HEAST) are constructed for use in the Superfund and RCRA programs but do not represent Agency-wide expert judgments. These tables are publicly available from the Superfund program. The tables include Slope Factors, Unit Risks, and WOE categorizations for chemicals with cancer effects, and RfDs and RfCs for noncancer effects.

**Derived Values.** For a prioritized group of chemicals for which sufficient data was not found in the above sources, a group of EPA expert health scientists reviewed other available data to derive appropriate toxicity weights. Although individual literature searches for toxicological and epidemiological data for each chemical were beyond the scope of this project, sources such as the Hazardous Substances Data Base (HSDB), as well as various EPA and ATSDR summary documents, provided succinct summaries of toxic effects and quantitative data, toxicological and epidemiological studies, and, in some cases, regulatory status data. When the available data on chronic human toxicity were sufficient to derive values, a toxicity weighting summary was developed summarizing the information used to develop each of these values. The summaries are available in Technical Appendix A. The EPA scientists use a technical approach analogous to the Agency's method for deriving RfD values, RfC values, cancer risk estimates, and weight-of-evidence (WOE) determinations. However, it must be emphasized that these derived values are not the equivalent of the more rigorous and resource-intensive IRIS process and are only useful for screening-level purposes.

Data from these sources are categorized in three-tiered, hierarchical fashion to give preference to EPA and consensus data sources, where possible. Data are gathered separately for individual endpoints; a chemical's RfD may be from IRIS, while its Oral Slope Factor may be from HEAST.

The hierarchy used in toxicity weighting is as follows:

**Tier 1**. The most recent data from IRIS and OPP is used for each chronic health endpoint. If the dates are comparable, preference is given to IRIS, since IRIS reflects Agency-wide judgments.

**Tier 2**. In the absence of data from the above sources for an individual chronic health endpoint, toxicity data from the most recent entry in ATSDR and CalEPA are used.

**Tier 3.** In the absence of data from the above sources for an individual chronic health endpoint, the following data sources, in this order, are used: 1) HEAST; 2) Derived; and 3) IRIS values previously used in toxicity weighting, that were withdrawn pending revision.

For chemicals with carcinogenicity risk values, weight-of-evidence (WOE) values are obtained using the same data source hierarchy. Therefore, preference is given to WOE's from IRIS or OPP. As a general rule, chemicals with cancer potency factors from IRIS or OPP will also have WOEs. CalEPA, however, references either EPA or the International Agency for Research on Cancer (IARC) for WOE designations. Therefore, in the absence of an EPA consensus WOE, WOE's are obtained from IARC. However, due to the differences in WOE definition, it is not always possible to translate IARC WOE's into EPA WOE's without examining the toxicity data. WOE's are matched in the following way:

- IARC Group 1 = EPA Group A (Human Carcinogen)
- IARC Group 2A = EPA Group B (Probable Human Carcinogen)
- IARC Group 2B = EPA Group B or EPA Group C (Possible Carcinogen)
- IARC Group 3 = EPA Group D (Not Classifiable as to Human Carcinogenicity)
- IARC Group 4 = EPA Group E (Evidence of Non-Carcinogenicity)

The IARC 2B designation is not easily translated to the EPA designation, because its definition spans EPA Groups B and C. This is a particularly important distinction because the use of a B2 or C designation will affect the calculation of the toxicity weight. Therefore, for the chemicals with IARC 2B designations, summaries of the toxicity data used to generate the oral slope factor or inhalation unit risk are evaluated to derive WOEs. To date, this approach has been used for chemicals with data from CalEPA; therefore, the CalEPA "Technical Support Document for Describing Available Cancer Potency Factors" was used for the background information.

Currently, using all of the available data sources described above, toxicity weights are available for 426 of 610 chemicals and chemical categories on the 2000 TRI Chemical List. Chemicals with toxicity weights account for over 98% of the reported pounds for all on-site releases in 2000. The Indicator Elements are recomputed for all years in the TRI database on an annual basis in order to incorporate revisions to the reporting data.

Toxicity weights for individual chemicals and chemical categories are presented in Technical Appendix A.

## 4.4 How Indicator Toxicity Weightings Differ from EPCRA Section 313 Criteria

As noted above, the model uses TRI chemical reporting data. All TRI chemicals included in the model are listed on the TRI because they meet one or more statutory criteria regarding acute or chronic human toxicity, or environmental toxicity. The goal of the RSEI model is to use these data reported to the Agency to investigate the relative risk-based impacts of the releases and transfers of these chemicals on the general, non-worker population. To achieve this goal, the model differentiates the relative toxicity of listed chemicals and ranks them in a consistent manner. The ranking of each chemical reflects its toxicity only relative to other chemicals that are included in the model. Toxicity is not compared to some benchmark or absolute value as is required when adding or removing a chemical from the TRI. Furthermore, the model addresses only the single, most sensitive chronic human health toxicity endpoint.

It is important that the public not confuse the use of the RSEI model as a screening-level tool for investigating relative risk-based impacts related to the releases and transfers of TRI chemicals,

with the very different and separate activity of listing/delisting chemicals on the TRI using statutory criteria. A description of the listing/delisting criteria and process is described below.

The Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) section 313(d)(2) sets out criteria for adding chemicals to the list of chemicals subject to reporting under EPCRA section 313(a). The statutory criteria used for listing and delisting chemicals addresses the "absolute" chronic toxicity of chemicals on the TRI (e.g., multiple effects or the severity of effects). For a chemical (or category of chemicals) to be added to the EPCRA section 313(c) list of toxic chemicals, the Administrator must judge whether there is sufficient evidence to establish any one of the following:

Acute Human Toxicity §313(d)(2)(A) - The chemical is known to cause or can reasonably be anticipated to cause significant adverse acute human health effects at concentration levels that are reasonably likely to exist beyond facility site boundaries as a result of continuous, or frequently recurring, releases.

**Chronic Human Toxicity** §313(d)(2)(B) - The chemical is known to cause or can reasonably be anticipated to cause in humans—

(i) cancer or teratogenic effects, or

- (ii) serious or irreversible-
  - (I) reproductive dysfunctions,
  - (II) neurological disorders,
  - (III) heritable genetic mutations, or
  - (IV) other chronic health effects.

**Environmental Toxicity** \$313(d)(2)(C) - The chemical is known to cause or can reasonably be anticipated to cause, because of—

(i) its toxicity,

(ii) its toxicity and persistence in the environment, or

(iii) its toxicity and tendency to bioaccumulate in the environment, significant adverse effect on the environment of sufficient seriousness, in the judgment of the Administrator, to warrant reporting under this section.

To remove a chemical from the section 313(c) list, the Administrator must determine that there is not sufficient evidence to establish any of the criteria described above as required by EPCRA section 313(d)(3).

The EPA examines all of the studies available for a chemical to decide if the chemical is capable of causing any of the adverse health effects or environmental toxicity in the criteria. Agency guidelines describe when a study shows such effects as cancer (EPA, 1986a), developmental toxicity (teratogenic effects) (EPA, 1991b), or heritable genetic mutations (EPA, 1986b). The

review makes a qualitative judgment regarding the potential of each chemical to meet at least one of the criteria and the chemical is added to the list if this judgment is positive. If a chemical is on the list and it is not possible to make a positive judgment regarding any of the criteria, then the chemical can be removed.

There is no correlation between the toxicity criteria and methodology used to make listing decisions under EPCRA section 313 and the methodology used to assign toxicity weights to chemicals for the RSEI model. Therefore, these toxicity weights cannot be used as a scoring system for evaluating listing/delisting decisions. RSEI also does not attempt to reflect the statutory criteria for these chemicals.

## 5. Exposure and Population Modeling

To estimate the magnitude of exposure potential from TRI releases, a separate exposure evaluation is conducted for each chemical release pathway. The following pathways are evaluated:

- **Air**: stack and fugitive pathways;
- **Surface Water**: drinking water intake and fish ingestion pathways;
- **Publicly-Owned Treatment Works (POTWs)**: fugitive air, groundwater (not currently modeled), drinking water intake and fish ingestion pathways;
- Land: groundwater pathway (not currently modeled), volatilization to air included in fugitive air emission pathway for on-site releases; and
- **Off-site transfers**: groundwater (not currently modeled), volatilization (not currently modeled) and stack air (from incineration) pathways.

The ideal derivation of a dose would involve a *site-specific* exposure assessment for each release and exposure pathway. However, such an effort is well beyond the scope of this project; further, reporting of extensive site-specific information relevant for exposure modeling is not part of a TRI data submission. For example, the EPA Form R (Toxic Release Inventory Reporting Form) does not require submission of data on groundwater flow, soil conditions, and other factors that affect groundwater contamination from land releases. Although some site-specific data are used in the model, it is not the intent of this project to gather extensive site-specific data or measurements that would be needed to perform site-specific calculations. The need to accurately reflect exposure characteristics in the RSEI model must be balanced by the need for simple and understandable results that are easily communicated to the public and that are based on currently available data.

Therefore, in this method, the exposure evaluations combine data on pathway and media-specific emission volumes, physicochemical properties and, where available, site characteristics, with models to determine an estimate of the ambient concentration of contaminant in the medium into which the chemical is released. The ambient media concentrations are then combined with human exposure assumptions to estimate a "surrogate dose". The term surrogate dose is used because limited facility-specific data and the use of models that rely on default values for many parameters preclude the calculation of an actual dose estimate. Instead, the purpose of the method is to generate as accurate a surrogate doses from releases of TRI chemicals are *comparable only to the surrogate doses resulting from other releases included in the model*.

Estimates of the surrogate dose for each potentially exposed person are combined with estimates of the number of people potentially exposed. Potential exposure is determined by the geographic location of the population, as identified by the U.S. Decennial Census for 1990 and for 2000. The size of the exposed population is calculated separately for each pathway. The model assumes continuous exposure, and does not account for the activity patterns of the people

potentially exposed. However, population estimates do consider changing demographic patterns (total population, as well as subpopulations by age and sex).

The methods used to model each type of release are specific to that type of release and depend on data available to evaluate that pathway. In some cases, models are combined with some sitespecific data to estimate exposure; in other cases, generic reasonable worst-case models may be used in the absence of any site-specific data. The physicochemical property data used for the exposure evaluation are found in Technical Appendix B. It should be noted, however, that products of decay are not modeled. Exclusion of these decay products from the model may underestimate or overestimate the risk impact of releases, since the decay product may be more or less toxic than the parent compound.

Specific pathway calculations are discussed in the sections below. First, Section 5.1 discusses the geographic basis of the model, and describes the grid cell system underlying the model and how facilities and people are located on it. This discussion describes how annual grid cell-level general population data sets are created. From these general population data sets, the model generates estimates of populations exposed through particular pathways. The next sections describe the modeling for each pathway, including the estimation of surrogate doses and exposed population for that pathway.

## 5.1 Geographic Basis of the RSEI Model

Underlying the RSEI method is the ability to locate facilities geographically, and to attribute characteristics of the physical environment, such as meteorology, to areas surrounding the facilities, once they are located. To accomplish the location of facilities and the attribution of data to those facilities, the model describes the U.S. and its territories as a 1-km by 1-km grid system. For each cell in the grid, a location "address" in terms of (X,Y) coordinates is assigned based on latitude and longitude (lat/long).

#### 5.1.1 The Model Grid Cell System

The grid cell system is based on a series of (X,Y) coordinates that locate the center point of each cell in the grid. Location is based on latitude and longitude, with the origin set at the intersection of the prime meridian and the equator. Therefore, each X and Y coordinate is defined as:

Х	=	distance to the prime meridian from a given latitude of Y (km), and
Y	=	distance from the equator, with North latitudes considered the positive
		direction (km).

The result is a series of cells that form a grid across the United States. Each cell approximates a 1-sq km area. The (X,Y) coordinates of the center of each cell from a given latitude and longitude are defined as follows:

$$X = INT(Rad*cos(LatR)*LongR) / Cell) + AdjustX$$
(Eq. 5.1)

$$Y = INT(LatD / YBand) + AdjustY$$
(Eq. 5.2)

where:

Rad	=	Earth's radius, 6366707.444 meters;
Cell	=	size of the grid cell: 1000 meters;
LatR	=	latitude of position in radians;
LongR	=	longitude of position in radians;
LatD	=	latitude of position in decimal degrees;
Yband	=	(180/(Radius * pi)) * CellSize;
AdjustX	=	0.5 if latitude $>0$ , -0.5 if latitude $<0$ ;
AdjustY	=	0.5 if longitude >0, -0.5 if longitude<0;

#### 5.1.2 Locating Facilities on the Grid

Once the grid system for the U.S. is created, each facility must be located on the grid, assigned to a grid cell. The grid cell assignment is based on the facility's latitude and longitude (lat/long) coordinates, using equations 5.1 and 5.2 above. Once a grid cell is assigned, the facility is assumed to be at the cell's center, for ease of modeling. For a complete description of the method used to select lat/long coordinates for both reporting facilities and off-site facilities, see Technical Appendix D.

**Reporting Facilities.** Because the location of a facility is key to the subsequent exposure modeling (e.g, facility location will determine which population is assumed to be exposed to its air releases), it is important that the lat/long coordinates are as accurate as possible. Each facility reporting to TRI is instructed on Form R to provide the lat/long coordinates of the facility, or, if the facility is large, the lat/long coordinates of a point central to the production activities of the facility. However, these reported coordinates vary widely in terms of their precision. Before

Version 2.1 January 2004 locating facilities on the model grid, a quality assurance (QA) procedure is performed to improve the data. The QA procedure compares the reported coordinates, other EPA locational data, and coordinates from a commercial geocoding service, <sup>6</sup> and selects the best set of coordinates according to a series of tests. Equations 5.1 and 5.2, which determine the (X,Y) coordinates of the grid cell centers are then used to transform facility lat/long coordinates to (X,Y) coordinates, and the facility is assigned to the grid cell with the same (X,Y) coordinates. The facility is then modeled as being located at the center of its assigned cell.

Off-site Facilities. RSEI also models some potential exposures that may result from environmental releases of chemicals from "off-site" facilities, that is, facilities that receive transfers from TRI-reporting facilities. Note that off-site facilities do not report transfers received from other facilities directly to TRI; instead their names and addresses are reported by the facilities that transfer chemicals to them.<sup>7</sup> Each report of a receiving off-site facility becomes a separate record in the TRI, even though each off-site facility often receives transfers from more than one TRI-reporting facility. This produces multiple records of the same off-site facility; however, because the names and addresses are not standardized, the records are usually slightly different, and so cannot easily be matched to each other. EPA has developed an approximate text string matching program to identify imperfect matches in order to collapse the set of off-site facilities to what are considered to be unique off-site facilities. The program matches values without requiring their exact equality. This approach accommodates misspelled words and inconsistencies in how a facility might report its identifying information over time. For example, "DuPont," "Du Pont" and "E.I. DuPont" might all refer to the same facility. A possible match is identified based on similarity rather than exact equality in the name field, and then the address fields are examined to determine whether the records match.

Approximate matching always introduces the possibility of error. Two records may be matched that do not in fact belong to the same unique facility. Generally, RSEI errs on the side of caution, and allows some number of duplicate records to remain in order to minimize the number of false matches made. Duplicate records have no negative consequences unless some of the unmatched records did not have assigned lat/long coordinates and so could not be located on the grid (see next paragraph). For the TRI Year 2000 data, the original database of approximately 3 million off-site facility records (including 1 million blank or not viable records and 1.7 million exact duplicates) was collapsed to less than 40,000 facilities.

<sup>&</sup>lt;sup>6</sup> Geocoding services were provided by Thomas Computing Services.

<sup>&</sup>lt;sup>7</sup> Some facilities may be considered both on-site and off-site facilities, if they both receive chemical transfers from other facilities (as an off-site facility) and emit reportable chemical releases (as an on-site facility). RSEI does not attempt to account for emissions that may be double-counted in this way.

Because off-site facilities do not report directly to TRI, and the reporting facilities only report the off-site facility's name and address, there is no lat/long data in TRI for off-site facilities. Using the original, non-collapsed data set (but after the blank and duplicate records were removed), the records were geocoded based on their reported address. The approximate matching program was run, resulting in groups of facility records determined to be matches. For each group, the record whose geocoded lat/long was of the highest confidence level was selected. The name, address and lat/long for this facility record is used in the model to represent all of the records in that matched group. In the same manner as for reporting facilities, Equations 5.1 and 5.2 are used to transform the lat/long coordinates to an (X,Y) cell address. The off-site facility is assumed to be in the center of its assigned grid cell.

#### 5.1.3 Locating People on the Grid

In order to estimate potential exposure, the U.S. population must also be geographically located on the model grid. To match annual TRI emissions and capture the effect of the changing distribution of the population, RSEI uses detailed annual population datasets at the grid cell level. The data is based on U.S. Decennial Census data, and includes information on population age and sex. In previous versions of the model, U.S. Census race categories were available for viewing on the map (although not for calculating results). However, due to complications arising from changes in race categorization for the 2000 Census, race categories are not available for viewing in the current version of the model. The following sections describe how the U.S. Census data is used to generate annual population estimates, and how the unit of analysis for the U.S. Census (the block) is translated into the unit of analysis for the model (the grid cell).

**U.S. Census Data.** The model uses U.S. Decennial Census data for 1990 and 2000 at the block level.<sup>8</sup> Census blocks are the smallest geographic area for which decennial census data are collected. Blocks are of varying size, formed by streets, roads, railroads, streams and other bodies of water, other visible physical and cultural features, and the legal boundaries shown on Census Bureau maps. In 1990, there were approximately 7 million census blocks. Due to boundary changes and increased resolution for highly populated areas, there were approximately 9 million blocks in the 2000 Census. Block-level data from the 1990 Census and the 2000 Census<sup>9</sup> are used to create detailed age-sex population groups for each of the census blocks in the U.S. for 1990 and for 2000. Because the U.S. Census presents data in slightly different

<sup>&</sup>lt;sup>8</sup> U.S. Census data and block shape files were provided by GeoLytics, Inc.

<sup>&</sup>lt;sup>9</sup> For 1990, not all of the variables were available at the block level. For those variables that were only available at the block group level, block group ratios were calculated and applied to the data available at the block level. For 2000, all of the required variables were available at the block level.

format, some data processing was necessary to create the following age-sex population groups used in the model:

- Males Aged 0 through 9 years
- Males Aged 10 through 17 years
- Males Aged 18 through 44 years
- Males Aged 45 through 64 years
- Males Aged 65 Years and Older
- Females Aged 0 through 9 years
- Females Aged 10 through 17 years
- Females Aged 18 through 44 years
- Females Aged 45 through 64 years
- Females Aged 65 Years and Older

For Puerto Rico, mapping limitations dictated the use of block group data rather than block level data for 1990 (shape files were not available at the lower level of resolution). However, block level data and shape files were used for 2000. For the U.S. Virgin Islands, American Samoa, Guam, and the Northern Mariana Islands, mapping was limited to whole-island areas or county equivalents, so the population data is also at this level of detail. Detailed demographic data were not available, so Census Bureau estimates of age and sex ratios for 2000 were used instead, and applied to actual 1990 and 2000 Census totals. The mapping to grid cells for Puerto Rico and island areas is the same as described below, except that the shape files are at various levels of geography rather than all at the block level.

**Mapping blocks to grid cells.** Because the grid cell is the unit of analysis for the model, Census data must be transposed from blocks to the model grid cells. Census provides the geometry for each block in the Topologically Integrated Geographic Encoding and Referencing (TIGER) geographic database, which was used to create shape files for the 1990 and the 2000 Census years. A corresponding set of shape files for grid cells was created, with each grid cell defined by its four corner points, calculated from its (X,Y) coordinates. The shape files were then compared, in essence overlaid, and each block was mapped to the cells in the grid that it overlaid, and the percentage of the block's total area falling within each cell was calculated.<sup>10</sup>

The process described above was performed separately for 1990 and 2000, as the block boundaries had changed between the Censuses. This process resulted in two tables, each with

<sup>&</sup>lt;sup>10</sup> Due to irregular, invalid block shapes, some of the block percentages did not sum to 100 percent. For these blocks, the boundary overlay process was not used; instead, the whole block was assigned to whatever grid cell contained the centroid of the block (an approximate center point defined by the Census). For 1990 Census data, the centroid method was used for 1,617 blocks out of almost 7 million populated Census blocks; for 2000, the centroid method was used for 182,901 out of approximately 8 million populated Census blocks.

four fields: the X coordinate and the Y coordinate which identify the grid cell, the block identifier assigned by the Census, and the percent of that block assigned to the grid cell.

**Calculating Populations.** For each block assigned to a grid cell, the block populations were multiplied by the percent of that block assigned to that grid cell. Those values were then summed over each grid cell. This process was performed separately for 1990 and 2000, resulting in two grid cell level datasets, each containing the ten age-sex population groups listed above.<sup>11</sup> For 1990, there were 6,116,345 populated grid cells; for 2000, there were 6,093,796. These datasets can be found in the model database as "Census90" and "Census00." To create annual datasets for 1991 through 1999, a straight-line interpolation at the grid cell-level is performed within the model between the two data sets. The line is extrapolated backward to create annual datasets for 1988 and 1989.

<sup>&</sup>lt;sup>11</sup> The data processing results in fractional people; populations were rounded to four decimal places for use in calculations, but are rounded to the nearest integer for display in the model.

### 5.2 Pathway-specific Methods to Evaluate Chronic Human Exposure Potential

The following sections describe the algorithms for modeling exposure for each of the following exposure pathways: (1) stack and fugitive air releases, (2) direct surface water releases, (3) transfers to POTWs, (4) off-site transfers, and (5) on-site land releases. An overview of the pathways and methods used to evaluate each pathway is presented in Exhibit 2.1.

The following discussions of exposure modeling frequently mention concentration and surrogate dose. This is not meant to imply that dose can be accurately calculated within this model. The exposure algorithms are intended to be simple ways to gauge relative risks from releases to different media in a consistent, defensible way, by modeling and estimating exposure. In some cases, the modeling is purposely simplified, given the lack of site-specific data.

When possible, exposures are estimated for relevant subpopulations defined by age, sex, or other factors. Exposure for individual subpopulations is modeled using exposure factors (i.e., inhalation rates, drinking water intakes, fish ingestion rates, and body weight) and population data specific to such subpopulations. For example, ingestion rates specific to recreational and subsistence fishers are used to estimate exposures for these fishers and their families. Also, age-and sex-specific inhalation and drinking water ingestion rates are used. The relevant exposure assumptions for these subpopulations are also described in the following sections.

## 5.3 Modeling Air Releases

Air releases accounted for approximately 18 percent of TRI emission by weight in 2000. Air releases can either be released through stacks or as fugitive releases. Stack (or point) air releases include releases to air through stacks, confined vents, ducts, pipes, or other confined air streams. Fugitive releases to air, which account for about 2 percent of all TRI emissions, include all other air releases, including leaks, evaporation from surface impoundments, and releases for building ventilation systems. These are modeled as two separate pathways in the model, although the potentially exposed population and human exposure assumptions are the same for both. The following sections describe the method and data sources for each pathway.

#### 5.3.1 Stack Air Emissions: Method

Stack air releases are modeled using algorithms from the Industrial Source Complex Long Term (ISCLT) model developed by EPA's 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 stack or area source. The pollutant concentration is a function of facility-specific parameters, meteorology, and chemical-specific, first-order air decay rates. The following sections describe the parameters of the ISCLT model used.<sup>12</sup>

#### 5.3.1.2 Model Dispersion Options

Since the ISC models are especially designed to support the EPA's regulatory modeling programs, the regulatory modeling options, as specified in the Guideline on Air Quality Models (Revised)<sup>13</sup>, are the default mode of operation for ISCLT and also for the ISCLT algorithms used within the model. These include algorithms for modeling the effects of stack-tip downwash, buoyancy-induced dispersion, final plume rise, and for processing averages when calm winds occur. [Stack-tip downwash algorithms account for the initial plume height being depressed when plume material is drawn down into the low pressure region of the stack wake. Buoyancy induced dispersion is the initial dispersion of plumes caused by turbulent motion of the plume and turbulent entrainment of ambient air.] The model also utilizes ISCLT default values for wind profile exponents and default values for vertical potential temperature gradients. The wind profile exponents are used to adjust the observed wind speed according to the wind power law (see Exhibit 5.2 and Equation 5.5). A further discussion of all regulatory modeling options is presented in Section 5.3.1.6 of this document.

Within the model, both rural and urban dispersion parameters are used. For facilities where the average population density in the surrounding 101-km by 101-km grid is greater than or equal to 750 persons per square mile, urban dispersion parameters are used. When the average population density in the surrounding grid is less than this, the model uses rural dispersion parameters.

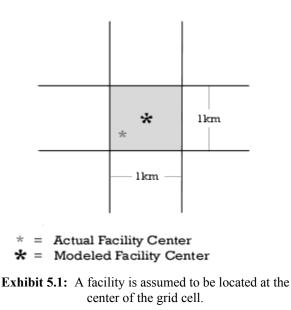
The effects of building downwash—aerodynamic wakes and eddies produced by plant buildings and structures on plume dispersion—are not considered in the model. This is principally because the model is designed to be used as a screening tool and because site-specific data like building location and size data are not readily available. However, not modeling building downwash is equivalent to assuming that facility stacks are designed according to Good Engineering Practice (GEP). When stacks are equal to or greater than the GEP height, it is not necessary to model building downwash effects (EPA, 1993b).

<sup>&</sup>lt;sup>12</sup> The following description is based on equations and text provided in the ISCLT manuals. The most recent ISCLT manuals are available from EPA's SCRAM website at http://www.epa.gov/scram001/.

<sup>&</sup>lt;sup>13</sup> The Guideline on Air Quality Models can be found in 40CFR Part 51, Appendix W or accessed online at: http://www.epa.gov/ttn/scram/guidance/guide/appw\_99.pdf.

#### 5.3.1.3 Source Parameters

In Version 2.1 of the model, the U.S.<sup>14</sup> is divided into a grid of 1 kilometer by 1 kilometer square grid cells. Facilities are assigned to a particular grid cell in this grid according to their latitude and longitude coordinates (see Technical Appendix D for details on the coordinates used). To increase modeling efficiency, a facility is then assumed to be located at the center of the grid cell, regardless of where its latitude and longitude coordinates place it within the cell (see Exhibit 5.1).



As a result of this assumption, the actual location of a facility may differ from its modeled location by up to 707 meters, the maximum distance between the center and the corner of the cell. To simplify the analysis, a facility's point source emissions are modeled as a single stack located at the facility's geographic center.

RSEI uses facility-specific stack parameters when available. These include stack height, exit-gas velocity, and stack diameter. Stack exit gas temperature is assumed constant for all stacks (293° K). For facilities with multiple stacks, the median value for the stack heights and diameters for

<sup>&</sup>lt;sup>14</sup> Including Puerto Rico, the U.S. Virgin Islands, American Samoa, Guam, and the Northern Mariana Islands.

that facility is used. For facilities without stack-specific values, a Standard Industrial Classification (SIC) code-based median stack parameter is assigned to the facility. If no valid SIC code is available, or no stack data is available for that SIC code, then overall median values are used. Stack parameters are discussed further in Section 5.3.5.1 and in Technical Appendix E.

Annual stack air releases as reported to TRI are converted to an equivalent constant emission rate in grams per second according to the following equation<sup>15</sup>:

$$Q = \frac{453.6 \ q}{31,536,000} \tag{Eq. 5.3}$$

where:

Q	=	pollutant emission rate (g/sec),
q	=	TRI annual stack or point air emissions (lb/yr),
453.6	=	constant to convert pounds (lb) to grams (g), and
31,536,000	=	constant to convert years (yr) to seconds (sec) assuming 365 days
		per year.

#### 5.3.1.4 Meteorological Input Data

For a given pollutant source, meteorology around the source affects the dispersion characteristics. Meteorological factors such as wind speed and direction, air temperature, stability, turbulence and the height of the mixing layer all have a direct effect on the dispersion and dilution of air pollution and the resulting magnitude and location of ground level concentrations of emitted pollutants.

The required meteorological input data for air modeling are annual STability ARray (STAR) summaries (as 25-year average frequency distributions). These are joint frequency distributions of wind speed class by wind direction sector and Pasquill atmospheric stability category. The Pasquill-Gifford Stability classification characterizes atmospheric stability into 6 classes: A, B, C, D, E, and F (or 1, 2, 3, 4, 5, and 6). Class A denotes the most unstable and hence most turbulent conditions, and Class F denotes the most stable or least turbulent conditions.

<sup>&</sup>lt;sup>15</sup> Although RSEI can model any chemical air emission that is accompanied by the appropriate locational, chemical, and toxicity weight information, the model currently uses Toxic Release Inventory (TRI) reporting as the source of chemical release information.

The model uses STAR summaries obtained from the National Climatic Data Center and additional STAR summaries for other locations generated using the STAR utility program available on EPA's SCRAM Bulletin Board<sup>16</sup>.

#### 5.3.1.5 The Gaussian Sector Average Equation

The emission rates from Equation 5.3 are used to determine the pollutant concentration at a distance r greater than one meter away from the facility stack. The concentration for a given chemical is calculated for each cell surrounding the stack using the radial distance of each grid cell's center from the source in the center cell, meteorological data, and chemical-specific data.

In the ISCLT algorithms, the area surrounding the facility stack is divided into sectors of equal angular width corresponding to the sectors of the annual frequency distributions of wind direction, wind speed, and stability (STAR data). Annual emissions for a point source are partitioned among these sectors according to the frequencies of wind blowing toward the sectors. The resultant average annual concentrations for each receptor point  $(r,\theta)$  calculated for a stack are then translated to the grid system coordinates used by the model.

For a single stack, the mean annual concentration is given by the following Gaussian sector average equation<sup>17</sup>:

$$C_{air,r_{ijk}} = \frac{K}{\sqrt{2\pi} r \Delta \theta} \cdot \Sigma_{ijk} \frac{Q f S V D}{u_{s} \sigma_{z}}$$
(Eq. 5.4)

where:

C <sub>air,r</sub> K r	= = =	mean annual air concentration at distance $r (\mu g/m^3)$ , 10 <sup>6</sup> , constant to convert (g) to ( $\mu g$ ), radial distance from stack (m),
$\Delta \theta$	=	sector width (radians),
i	=	integer indicating the i <sup>th</sup> wind-speed category (from STAR data),
j	=	integer indicating the j <sup>th</sup> wind-direction category (from STAR data),
k	=	integer indicating the k <sup>th</sup> atmospheric stability category (from STAR data),
Q	=	pollutant emission rate (g/sec),

<sup>&</sup>lt;sup>16</sup> EPA's SCRAM bulletin board can be found on the world wide web at http://www.epa.gov/scram001/.

<sup>&</sup>lt;sup>17</sup> This equation is from EPA (1992b), and is specific to a given wind speed, direction, and atmospheric stability category (*ijk*). Each facility has several combinations of these parameters for each distance (r) that must be summed to arrive at total concentration at that distance from the plant.

f	=	frequency of occurrence of the ith wind-speed category, the jth wind-
		direction category and the k <sup>th</sup> stability category (dimensionless),
S	=	smoothing function used to smooth discontinuities at sector boundaries
		(dimensionless),
V	=	vertical term (dimensionless),
D	=	term for pollutant-specific decay term in air, where $D = e^{r^* Kair/u^* 3600}$ , $K_{air} =$
		decay rate in air $(hr^{-1})$ , r = downwind distance (m), and $3600 = constant$ to
		convert (hr) to (sec),
u,	=	mean wind speed at the stack height (m/sec), and
$\sigma_{z}^{s}$	=	standard deviation of vertical concentration distribution (m).
Z		

The mean wind speed  $(u_s)$  at the stack height  $(h_s)$  is adjusted using the observed wind speed from the STAR summaries  $(u_{ref})$  according to the wind power equation:

$$u_s = u_{ref} \cdot \left(\frac{h_s}{z_{ref}}\right)^p$$
(Eq. 5.5)

where:

u <sub>s</sub>	=	mean wind speed at the stack height (m/sec),
u <sub>ref</sub>	=	wind speed at the measurement height (m/sec),
h <sub>s</sub>	=	stack height,
Z <sub>ref</sub>	=	reference height at which wind speed was measured (m), and
р	=	wind profile exponent (a function of Pasquill atmospheric stability
		category. See Exhibit 5.2).

#### Exhibit 5.2 Wind Profile Exponents

Stability Category	Rural Exponent	Urban Exponent
А	0.07	0.15
В	0.07	0.15
С	0.10	0.20
D	0.15	0.25

Stability Category	<b>Rural Exponent</b>	Urban Exponent
Е	0.35	0.30
F	0.55	0.30

The vertical term (V) accounts for the vertical distribution of the plume. It includes the effects of plume rise, limited mixing in the vertical, gravitational settling, and dry deposition of particulates.

Equations that approximately fit the Pasquill-Gifford stability curves are used to calculate the lateral dispersion of the concentration distribution ( $\sigma_z$ ) according to the following equation:

$$\sigma_z = a r^b$$
 (Eq. 5.6)

where:

$\sigma_z$	=	standard deviation of vertical concentration distribution (m),
a,b	=	coefficients based on Pasquill-Gifford Stability category, and
r	=	distance downwind of the stack (km).

#### 5.3.1.6 Regulatory Default Options

As mentioned earlier, the standard regulatory modeling options for ISCLT are used within the model. These regulatory modeling options are specified in the Guideline on Air Quality Models (Revised).

The calculation for stack-tip downwash is a function of stack height, stack exit gas velocity, and stack diameter. In order to consider stack-tip downwash, the physical stack height is modified according to the following equation:

= 
$$h_s$$
 for  $v_s \ge 1.5u_s$   
or (Eq. 5.7)

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1988-2000 TRI data

$$h_{s}^{'} = h_{s} + 2d_{s} \left[\frac{v_{s}}{u_{s}}\right] \text{ for } v_{s} < 1.5u_{s}$$

where:

h	=	modified physical stack height (m),
h <sub>s</sub>	=	physical stack height (m),
d <sub>s</sub>	=	stack diameter (m),
V <sub>s</sub>	=	exit gas velocity (m/s), and
u <sub>s</sub>	=	stack height wind speed (m/s).

With regulatory defaults in effect, the model also incorporates the effects of buoyancy-induced dispersion, the initial dispersion of plumes caused by turbulent motion of the plume and entrainment of ambient air. Buoyancy-induced dispersion affects both the vertical and lateral spread of the concentration distribution. The effective vertical dispersion ( $\sigma_{ze}$ ) is calculated as follows:

$$\sigma_{ze} = \sqrt{\sigma_z^2 + (\frac{\Delta h}{3.5})^2}$$
(Eq. 5.8)

where:

$\sigma_{ze}$	=	the effective vertical dispersion of the plume (m),
$\sigma_{z}$	=	the vertical dispersion due to ambient turbulence (m), and
∆h	=	the plume rise due to momentum and/or buoyancy.

The lateral plume spread  $(\sigma_{ve})$  is parameterized in a similar fashion.

The model also incorporates the effects of final plume rise. Plume rise (the final plume height) is a function of both buoyancy and the momentum fluxes of the plume. For most plume rise situations, the value of the Briggs buoyancy flux parameter,  $F_b (m^4/s^3)$  is needed. The Briggs buoyancy flux parameter is given by the following equation:

$$F_b = g v_s d_s^2 (\frac{\Delta T}{4T_s})$$
 (Eq. 5.9)

1988-2000 TRI data

Version 2.1 January 2004 where:

F <sub>b</sub>	=	Briggs buoyancy flux parameter (m <sup>4</sup> /s <sup>3</sup> ),
g	=	acceleration due to gravity (constant),
Vs	=	exit gas velocity (m/s),
d <sub>s</sub>	=	stack diameter (m), and
${\bigtriangleup}T$	=	$T_s - T_a$ , $T_s$ is the stack gas temperature (K), and $T_a$ is the ambient air
		temperature (K).

For determining plume rise due to momentum of the plume, the momentum flux parameter,  $F_m$  (m<sup>4</sup>/s<sup>3</sup>) is calculated by the following equation:

$$F_m = v_s^2 d_s^2 \left(\frac{T}{4T_s}\right)$$
(Eq. 5.10)

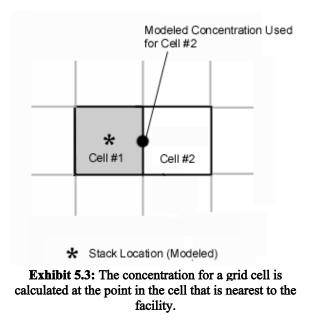
where:

F <sub>m</sub>	=	momentum flux parameter (m <sup>4</sup> /s <sup>3</sup> ),
Vs	=	exit gas velocity (m/s),
d <sub>s</sub>	=	stack diameter (m), and
ΔŤ	=	$T_s - T_a$ , $T_s$ is the stack gas temperature (K), and $T_a$ is the ambient air
		temperature (K).

The difference between the stack gas and the ambient air temperature determines whether buoyancy or momentum dominates. The interested reader is encouraged to consult the ISCLT User's Guide: Description of Model Algorithms for further explanation of the conditions during which buoyancy or momentum dominates.

#### 5.3.1.7 Calculating Pollutant Concentration

Using the equations described in the previous sections, the model calculates air concentrations at hypothetical "receptors" located within a 101-km by 101-km grid surrounding each facility. The model calculates ground-level concentrations at 1 kilometer increments for distances from 0.5 to 9.5 km away from the modeled facility, and at 4 kilometer increments from 9.5 to 49.5 km away. The concentration assigned to a given grid cell is determined at the point in that cell which is nearest to the facility (see Exhibit 5.3).



To estimate the concentration for the 1-km by 1-km center cell containing the facility, the model takes the arithmetic mean of the concentrations in 441 smaller (2500 m<sup>2</sup>) cells which make up the center cell. This methodology represents a change from previous versions of the model which did not directly model the concentration in the center cell. Prior versions of the model assigned the greatest concentration calculated in the 8 surrounding cells to the center cell. This change was instituted when analyses using the ISCLT model indicated that using the concentration in a surrounding cell as an estimate for the center cell may either significantly over or under-represent chemical concentrations there (See Part B of *Analyses Performed for the Risk-Screening Environmental Indicators*).

The maximum modeled east/west and north/south distances of 50 km replaces the 10 km distances used in previous versions of the model. This change was instituted to more adequately capture potential impacts of certain chemicals, and to account for increased stack height associated with reporting from electric utilities. To test the effects of changing modeled distances on results, EPA modeled air concentrations for the 20 most toxic carcinogens and the 20 most toxic non-carcinogens included the model at various stack heights. These analyses indicated that extending modeled distances to 50 kilometers was necessary to capture potential concentrations of concern under certain atmospheric conditions. This distance is expected to capture the majority of the potential impacts from the TRI facilities and chemicals. Details of these analyses can be found in Part B of *Analyses Performed for the Risk-Screening Environmental Indicators*.

#### 5.3.2 Fugitive Air Releases: Method

As for stack air releases, long-term pollutant concentrations downwind of the facility due to TRIreported fugitive air releases are modeled using algorithms from the Industrial Source Complex Long Term (ISCLT) Area-Source model. The model is based on a numerical integration over the area in the upwind and crosswind directions of a Gaussian point source plume formula (see Equation 5.4).

#### 5.3.2.1 Model Dispersion Options

Model dispersion options used in modeling fugitive air releases are the same as those used for stack air releases, as described in Section 5.3.1.2.

#### 5.3.2.2 Source Options

Fugitive emissions are modeled as an area source which is 10 meters by 10 meters in size, located at the center of the cell containing the facility. The model assumes a release height of 3 meters.

Fugitive emissions are converted from pounds per year to grams per square meter per second  $(g/m^2s)$  according to the following equation:

$$Q_a = \frac{453.6 \ q_a}{31,536,000 \ * \ 10^2}$$
 (Eq. 5.11)

where:

Q <sub>a</sub>	=	pollutant area emission rate (g/m <sup>2</sup> s),
$q_a$	=	TRI annual fugitive air emissions (lb/yr),
453.6	=	constant to convert pounds (lb) to grams (g),
31,536,000	=	constant to convert years (yr) to seconds (sec), and
$10^{2}$	=	conversion factor necessary to convert annual emissions (g/s) to
		area emission rate $(g/m^2s)$ , assuming an area 10 m x 10 m.

The ground-level pollutant concentration resulting from emissions by an area source is given by a double integral in the upwind (x) and crosswind (y) directions:

$$X = \frac{Q_a K}{2\pi\mu_s} \int_x \left(\frac{VD}{\sigma_y \sigma_z} \int_y \exp[\frac{-0.5y^2}{\sigma_y^2}] dy\right) dx \qquad (Eq. 5.12)$$

where:

,
d

#### 5.3.2.3 Calculating Pollutant Concentration

Pollutant concentrations are calculated in the same way for fugitive air releases as for stack air releases, as described above in Section 5.3.1.7.

## 5.3.3 Calculating Surrogate Dose for Air Releases

The calculated air concentrations described earlier are combined with assumptions regarding inhalation rate and human body weight to arrive at a surrogate dose for a given cell:

$$DOSE_{air} = \frac{C_{air} \bullet I_{air}}{BW} \bullet \frac{1}{1000}$$
(Eq. 5.13)

where:

DOSE <sub>air</sub>	=	surrogate dose of contaminant from air (mg/kg-day),
C <sub>air</sub>	=	air concentration in cell ( $\mu$ g/m <sup>3</sup> ),
I <sub>air</sub>	=	inhalation rate $(m^3/day)$ ,
BW	=	human body weight (kg), and
1000	=	constant to convert ( $\mu g$ ) to (mg).

Version 2.1 January 2004 1988-2000 TRI data

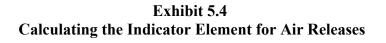
If the total population in the modeled area (the 10,201 cells in the 101 km by 101 km area surrounding the facility) is less than 2,953,971 persons, ISCLT automatically calculates air concentrations in the rural mode.

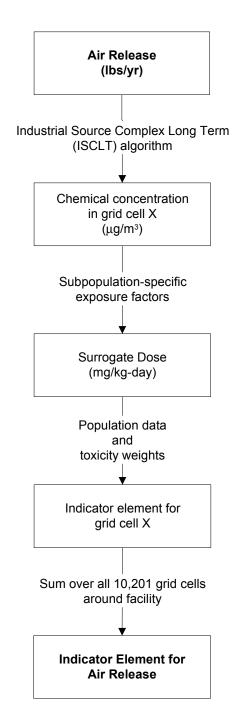
## 5.3.4 Estimating Population Size for Air Releases

The population potentially exposed to air releases is assumed to be equal to the population assigned to the grid cells in the 101 by 101 km modeled area, as described above in Section 5.1.3. Exposed population is only considered for grid cells with nonzero pollutant concentrations.

## 5.3.5 Calculating an Indicator Element for Air Releases

Exhibit 5.4 provides a graphical overview of the steps for determining the air modeling component of the model. First, the pollutant concentration in each cell is calculated using TRI emissions data and the ISCLT algorithms. Then, subpopulation-specific exposure factors are used to calculate a surrogate dose for each cell. Finally, the surrogate dose is multiplied by the number of people in each subpopulation in the cell and by the chemical toxicity weight. Then the results for all grid cells are summed. The result is an Indicator Element for air.





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## 5.3.6 Stack and Fugitive Air Releases: Data

The air pathways use facility-specific values (stack height, stack diameter and exit gas velocity), meteorology, chemical-specific first-order air decay rates, and exposure assumptions (inhalation rate and body weight). The values used for these pathways are summarized in Exhibit 5.5.

Parameter	Value	Source/Comment	
Pollution emission rate	Site-specific (lbs/yr)	TRI	
Stack height	Varies based on the facility and the availability of information. If available, the median height of all stacks at the facility is used. Otherwise one of the following is used in declining order of preference: the median stack height for the facility's 3-digit SIC code, the median stack height for the facility's 2-digit SIC-code, or the median stack height for all TRI-reportable SIC codes.	AFS, NET, EPRI (for Electric Utilities) and databases for CA, NY, and WI; these data are used in the vertical term of the model	
Stack diameters	Varies based on the facility and the availability of information. If available, the median diameter of all stacks at the facility is used. Otherwise one of the following is used in declining order of preference: the median stack diameter for the facility's 3-digit SIC code, the median stack diameter for the facility's 2-digit SIC- code, or the median stack diameter for all TRI-reportable SIC codes.	AFS, NET, EPRI (for Electric Utilities) and databases for CA, NY, and WI	
Exit gas velocity	Varies based on the facility and the availability of information. If available, the median exit gas velocity of all stacks at the facility is used. Otherwise one of the following is used in declining order of preference: the median exit gas velocity for the facility's 3-digit SIC code, the median exit gas velocity for the facility's 2-digit SIC- code, or the median exit gas velocity for all TRI- reportable SIC codes.	AFS, NET, EPRI (for Electric Utilities) and databases for CA, NY, and WI	
Exit gas temperature	293° K	EPA (1992b)	
Frequency of wind speed and direction	Site-specific	Wind stability arrays (wind-roses) derived from surface weather stations (NCDC Surface Airways Data)	

Exhibit 5.5 Air Modeling Parameters

Parameter	Value	Source/Comment	
Wind speed	site-specific (m/s)	Derived from surface weather stations (NCDC Surface Airways Data)	
Decay rate	Pollutant-specific values account for removal by physical and chemical processes (s <sup>-1</sup> )	SRC (1994-1999)	
Area source size	10 m <sup>2</sup>	EPA (1992b)	
Area source height	3 m	EPA (1992b)	

#### 5.3.6.1 Stack Height, Stack Diameter, and Exit Gas Velocity

Stack parameter data (height, diameter, and exit-gas velocity) were obtained from the AIRS Facility Subsystem (AFS) within the Aerometric Information Retrieval System (AIRS), the National Emission Trends (NET) Database, and databases from three individual states (California, New York, and Wisconsin). For each TRI facility that had stack parameter data in one or more of these sources, the median parameter of all stacks at the facility is used. For the TRI facilities that had no stack parameter data in these sources, the median parameter values for all of the facilities in that facility's Standard Industrial Classification (SIC) code is used instead. The SIC code-based stack parameters are estimated from data in AFS and the NET Database for facilities in the appropriate 3-digit SIC code, or in the 2-digit SIC code if the 3-digit SIC code is unavailable. If no 2-digit SIC code is available, the median of all stack parameters with TRIreportable SIC codes is used.

The Electric Power Research Institute (EPRI) provided EPA with site-specific data for electric utilities (electric utility SIC codes were added to TRI for Reporting Year 1998), transmitted in two databases. These data included stack height, stack diameter, and exit-gas velocity. Of the approximately 600 TRI facilities classified in one of the three electric utility SIC codes (4911-Electric Services; 4931-Electric and Other Services Combined; or 4939-Combination Utilities, not elsewhere classified), almost 70 percent matched a corresponding facility listed in one of the EPRI databases; approximately 30 percent of TRI electric utility facilities did not<sup>18</sup>. For the 30 percent that did not match specific facilities, the median parameters taken across all of the coal or oil combusting stacks in the EPRI databases were used.

<sup>&</sup>lt;sup>18</sup> One TRI facility classified in one of the relevant utility SIC codes that could not be matched to a specific facility in the EPRI dataset was matched to a specific facility in the AFS database. In this case, the facility-specific parameters were taken from AFS.

Statistical analysis of stack heights by SIC code revealed that for certain SIC codes, no significant height differences existed between stacks emitting TRI chemicals and those not emitting TRI chemicals. For these SIC codes, the median stack height was based on stack heights for all facilities. For SIC codes in which there were significant height differences between stacks emitting or not emitting TRI chemicals, only those stacks emitting TRI chemicals were used to calculate the median stack height for that SIC code.

For both stack diameter and exit gas velocity, the model uses the same data sources, criteria, and statistical methods described above for stack height data. Specifically, the model uses either the median value of all stacks for TRI facilities with this information or an SIC code-based median value for facilities without the appropriate stack data. Exit gas velocity data were obtained from AFS, NET, and state-specific databases. Stack diameter data were obtained from AFS, NET, EPRI and databases from three individual states (California, New York, and Wisconsin).

Analyses have been conducted that show air concentrations predicted by the model using a combination of generic and site-specific data closely match concentrations estimated by using more complete site-specific data. See Technical Appendix E for details on the derivation of stack data.

### 5.3.6.2 Meteorology

Weather data used in the model include wind speed, wind direction, and atmospheric stability. The source of these data are STability ARray (STAR) data, which are available from 420 weather stations throughout the U.S. For other weather stations which record hourly surface wind data, STAR data sets can be generated using the STAR utility program available on EPA's SCRAM Bulletin Board.<sup>19</sup> The STAR data set from the weather station closest to the facility is selected by the model as the input for the ISCLT algorithms.

In the STAR data set, wind speeds are divided into six classes: 0-3 knots; 4-6 knots; 7-10 knots; 11-16 knots; 17-21 knots; and greater than 21 knots. Pasquill-Gifford atmospheric stability classes A through F are characterized by wind speed, insolation, and cloudiness. These are summarized in Exhibit 5.6.

For any given combination of atmospheric stability category and wind speed class, the frequency of wind from each of the sixteen wind direction categories can be summarized in a "wind rose," a directional representation of this frequency. These frequency distributions may be on a monthly, seasonal, or annual basis. The STAR data currently used in the model are an average frequency distribution based on 25 years of meteorological data.

<sup>&</sup>lt;sup>19</sup> EPA's SCRAM bulletin board can be found on the world wide web at http://:www.epa.gov/scram001/.

		Insolation <sup>1</sup>			Nighttime Cloudiness <sup>2</sup>	
Surface wind speed <sup>3</sup> (m/sec)	Surface wind speed <sup>3</sup> (knots)	strong	moderate	slight	thinly overcast or ≥4/8 low cloud cover	≤3/8 cloud cover
<2	<3.8	А	A-B	В	-	-
2-3	3.9-5.8	A-B	В	С	Е	F
3-5	5.8-9.7	В	B-C	С	D	Е
5-6	9.7-11.7	С	C-D	D	D	D
>6	>11.7	С	D	D	D	D
	(for A-B, take the average of values for A and B, etc.)					

Exhibit 5.6 Atmospheric Stability Categories

1. Strong insolation corresponds to sunny midday in midsummer in England; slight insolation to similar conditions in midwinter.

2. Cloudiness is measured for the period from one hour before sunset to one hour after sunrise.

3. The neutral category D should also be used, regardless of wind speed, for overcast conditions during day or night and for any sky conditions during the hour preceding or following night as defined above. Source: Boubel et al., 1994.

4. 1 Knot = 0.51440 m/sec

#### 5.3.5.3 First-Order Air Decay Rates

Pollutants may be removed from the atmosphere by either physical processes or chemical transformation. The model uses pollutant-specific air decay rates from SRC's Atmospheric Oxidation Program (AOPWIN), an atmospheric oxidation computer program (SRC, 1994-1998). AOPWIN estimates the second-order rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals.<sup>20</sup> The daughter products of photodegradation are not modeled further, i.e., it is assumed that all chemicals are photodegraded into nontoxic compounds. AOPWIN data also contains certain empirically derived air decay rates. For the model, a concentration of hydroxyl radicals of  $1.5 \times 10^6$  molecules/cm<sup>3</sup> is used to convert the second-order rate constant provided in AOPWIN to a first-order rate constant. Furthermore, the rate is divided by a factor of two to reflect an assumed average day length of 12 hours:

<sup>&</sup>lt;sup>20</sup> For a few chemicals, other sources were used. See Technical Appendix B for the source used for each chemical.

$$K_{air} = \frac{AOPWIN}{2} * 1.x10^6 * 3600$$
 (Eq. 5.14)

where:

K <sub>air</sub>	=	air decay rate (hr <sup>-1),</sup>
AOPWIN	=	second-order rate constant from AOPWIN,
$1.5 \times 10^{6}$	=	hydroxyl radical concentration (molecules/cm <sup>3</sup> ),
3600	=	constant to convert molecules/seconds to molecules/hour, and
2	=	constant to reflect assumed day length of 12 hours.

#### 5.3.6.4 Human Exposure Data and Assumptions

For the air pathways, sex- and age-specific inhalation rates and body weights are used in the model. The primary source for all exposure factors used in the model is EPA's Exposure Factors Handbook (EPA, 1997b, hereafter denoted as EFH), which provides a summary of the available statistical data on various factors used in assessing human exposure. These factors include: drinking water consumption, soil ingestion, inhalation rates, dermal factors including skin area and soil adherence factors, consumption of fruits and vegetables, fish, meats, dairy products, homegrown foods, breast milk intake, human activity factors, consumer product use, and residential characteristics. In EFH, EPA recommends mean values for the general population and also for various segments of the population who may have characteristics different from the general population. RSEI uses inhalation rates and body weights derived from the recommended factors, except where noted. The Exposure Factors Handbook (EFH) can be found on the internet at http://www.epa.gov/ncea/exposfac.htm.

EFH (EPA, 1997b, Table 5-23, p. 5-24) was used to estimate inhalation rates for the eight RSEI age-sex groups (ages 0-17, 18-44, 45-64, 65+).<sup>21</sup> The inhalation rates recommended by EFH were not categorized into the same age groups used in RSEI. For children, the RSEI age groups were broader than the EFH age groups. Therefore, the exposure factor was calculated using a weighted average of the inhalation rates for all EFH age groups that overlap the RSEI age group as follows:

<sup>&</sup>lt;sup>21</sup> The RSEI model provides the ability to view risk scores for the 0-9 year old age group, however, there is not a separate exposure factor for this age group. Instead, the exposure factor for the 0-17 year old age group is used.

$$EF = \frac{\sum_{i} (IR_i \times n_i)}{N}$$
(Eq. 5.15)

where:

EF	=	RSEI exposure factor,
$IR_i$	=	intake rate for EFH age group <i>i</i> ,
n <sub>i</sub>	=	number of years that EFH age group <i>i</i> overlaps with the RSEI age
		group, and
Ν	=	number of years in RSEI age group.

For adults, EFH provides only a single recommended inhalation rate for males and a single rate for females. However, EFH also provides the underlying data used to develop the summary values, which were available for more narrow age ranges (EPA, 1997b, Tables 5-11 to 5-13, p. 5-13 to 5-15). The RSEI adult inhalation factors are based on weighted averages calculated from this data, using Equation 5.15. The RSEI inhalation factors are then divided by age- and sexspecific body weights, averaged to match the RSEI age groups using data provided in EFH (EPA, 1997b, Tables 7-2 and 7-3, p. 7-4). Exhibit 5.7 provides the range of data used, and Exhibit 5.8 presents the final exposure factors used in the model. More detail on the derivation of exposure factors can be found in Technical Appendix C.

**Exhibit 5.7 Range of Data Used to Estimate Exposure Factors** 

Parameter	Value	Source/Comment
Inhalation rate	4.5-17 m <sup>3</sup> /day (Varies by age and sex)	EPA (1997b)
Body weight	33.0 -79.9 kg (Varies by age and sex)	EPA (1997b)

Model Age Group	Male	Female
0-17	0.341	0.310
18-44	0.209	0.186
45-64	0.194	0.165
≥65	0.174	0.153

#### Exhibit 5.8 Inhalation Exposure Factors (m<sup>3</sup>/kg-day)

#### 5.4 Modeling Surface Water Releases

In 2000, approximately two percent of TRI emissions by weight were released on-site as direct surface water releases. People may be exposed to chemicals released into surface water in one of two ways: by drinking tap water from a public water system whose water intake was located in the stream path of a chemical release; or by eating contaminated fish caught in a water body in the stream path of a chemical release. The following sections first describe the methods used to calculate the initial stream concentration for both pathways, and then the different methods used to calculate surrogate dose and population for the drinking water pathway and the fish ingestion pathway. The data section presents the data used for both pathways and the human exposure assumptions used.

#### 5.4.1 Surface Water Releases: Methods

The first step in assessing surface water emissions is to locate the discharging facility on the grid. Facilities are then matched to a receiving stream reach (a linear, unbranched section of a water body). Facilities are assumed to discharge to the nearest reach, as long as that reach is within six kilometers of the facility. If no reach is found within six kilometers, the discharge is not modeled. Reach data is not available for Alaska, Hawaii, Puerto Rico, the U.S. Virgin Islands, Guam, American Samoa and the Northern Mariana Islands; therefore, no surface water releases are modeled for these areas.

Chemical concentrations in the receiving stream at a distance *x* from the discharging facility at time *t* are estimated by using a simple first-order decay equation. The facility is assumed to release its annual discharge at a constant rate throughout the year. Annual average concentrations are then estimated for distances up to 200 km downstream from the chemical release. Within the initial stream reach, the mass of the release is assumed to be instantaneously mixed with the flow at the upstream end of that reach. The calculated concentration at the downstream end of the reach is then converted back to a mass (after any decay) and the process is repeated in the adjoining reach. Reaches are defined by intersections with other hydrological features and these "nodes" initiate the next reach segment. The chemical-specific decay coefficient is predominantly based on abiotic hydrolysis or microbial biodegradation, but may also include photooxidation. The general form of the first-order decay equation is as follows:

$$C_x = C_0 e^{-k_{water}t}$$
(Eq. 5.16)

Version 2.1 January 2004 where:

$C_x$	=	concentration at distance x meters from the facility release point
		(mg/L) (up to 200 kilometers from release point),
$C_{ heta}$	=	initial concentration (mg/L), which equals chemical release
		(mg/day) divided by harmonic mean flow (see Eq. 5.24),
k <sub>water</sub>	=	decay coefficient (sec <sup>-1</sup> ), and
t	=	time at which $C_x$ occurs (sec), which equals $x/u$ , where u is the
		water velocity (m/sec).

For surface water releases, the RSEI model estimates chronic human health exposures for two pathways: drinking contaminated water and eating non-commercial contaminated fish. Methods used to estimate each of these exposures are described below.

#### 5.4.1.1 Modeling the Drinking Water Pathway

Surrogate doses from drinking water are calculated using the chemical concentrations in stream reaches where drinking water intakes are located. Drinking water intakes are located using their lat/long coordinates from the Safe Drinking Water Information System (SDWIS), and are assumed to be drawing water from the stream reach nearest to their plotted location. For this exposure pathway, the chemical concentration in drinking water is assumed to be equal to the stream concentration (calculated at the upstream end of the reach; conservatively using the highest concentration), up to the level of the Maximum Contaminant Level (MCL),<sup>22</sup> where applicable. (Seventy-three TRI chemicals had existing MCLs in effect during one or more years for which TRI data are available<sup>23</sup>; this number includes chemical categories that are treated as their elemental forms). If the stream concentration exceeds the MCL, the drinking water is assumed to be treated to the level of the MCL for the year of that release. For each stream reach with a drinking water intake, the chemical concentration is combined with standard exposure parameters (see Section 5.4.3.6) to yield a surrogate dose:

<sup>&</sup>lt;sup>22</sup> Copper and lead have action levels instead of MCLs; however, RSEI models them in the same manner as MCLs. This also applies to copper compounds and lead compounds, as metal compounds are modeled like their elemental forms.

<sup>&</sup>lt;sup>23</sup> As MCLs are sometimes revised and new ones have been added since TRI began reporting, RSEI applies MCL limits for only the years that the MCLs were in effect. For several chemicals for which MCLS were first instituted in 1976 and then revised in 1991, the original MCL values were not readily available, so the revised values were also used for the years before the revision. These chemicals are barium, cadmium, chromium, lead, lindane, mercury, methoxychlor, nitrate, selenium, and toxaphene.

$$DOSE_{dw} = \frac{C_{water,reach} \cdot I_{water}}{BW}$$
 (Eq. 5.17)

where:

$DOSE_{dw}$	=	surrogate dose of chemical in drinking water (mg/kg-day),
$C_{water,reach}$	=	average annual chemical concentration in the reach of interest,
,		calculated at the upstream end of the reach (mg/L),
I <sub>water</sub>	=	drinking water ingestion rate (L/day), and
BW	=	human body weight (kg).

#### 5.4.1.2 Estimating Population Size for the Drinking Water Pathway

To estimate the size of the population exposed to TRI releases through drinking water, the model uses estimates of the population served by each drinking water intake from the Safe Drinking Water Information System (SDWIS). (More information about SDWIS can be found at http://www.epa.gov/enviro/html/sdwis/sdwis\_ov.html.) However, this data set only lists the intake location and the number of people served by the water system. In many cases, there are multiple water intakes per water system. In the absence of other data, it is assumed that the total population of the water system is exposed to the full concentration of the released chemical estimated at the reach where a water intake is located (calculated at the upstream end of the reach).

The drinking water intake information from SDWIS contains only the number of people served by each drinking water system; it does not provide demographic or locational information for those served (the time frame in which this information was collected also varies widely). To derive demographic information (that is, age and sex breakdowns) for the population served, RSEI uses the percentage of people in each of the ten age-sex categories for the total population located in grid cells within an 80-km radius of each reach containing a drinking water intake (this information is calculated for the fish ingestion pathway - see Section 5.4.1.4). Then, these percentages are applied to the SDWIS intake population (population served), creating the subpopulation groups that are used for calculating results. For drinking water intakes without lat/long data (where the population served is apportioned to reaches in a county - see Section 5.4.3.2), the population demographics are determined for every reach in the county (as if there was an intake located on every reach).

#### 5.4.1.3 Modeling the Fish Ingestion Pathway

A second potential exposure pathway is through consumption of fish contaminated by chemicals discharged from TRI reporting facilities. These fish may be consumed by recreational and subsistence fishers and their families.<sup>24</sup> For stream reaches up to 200 km downstream from the facility, the chemical concentration in fish is estimated using the following equation:

$$C_{fish,reach} = C_{water,reach} \cdot BCF$$
 (Eq. 5.18)

where:

$C_{fish, reach}$	=	concentration in fish in the specified stream reach (mg/kg),
$C_{water, reach}$	=	average annual chemical concentration in the reach of interest
,		(mg/L), and
BCF	=	bioconcentration factor for chemical (L/kg).

The chemical concentration in fish in a reach is combined with exposure assumptions to determine the surrogate dose from this pathway:

$$DOSE_{f,c} = \frac{C_{fish,reach} \bullet I_{fish,pop}}{BW}$$
(Eq. 5.19)

where:

$DOSE_{f,c}$	=	surrogate dose of chemical c from facility $f(mg/kg-day)$ ,
$C_{fish, reach}$	=	average annual chemical concentration in fish tissue (mg/kg),
I <sub>fish, pop</sub>	=	fish ingestion rate for recreational or subsistence fishers (kg/day),
		and
BW	=	human body weight (kg).

#### 5.4.1.4 Estimating Population for the Fish Ingestion Pathway

The model uses several steps to estimate the population within each grid cell that consumes noncommercial fish. First, a county-level dataset containing the number of fishing or hunting/fishing combination licenses was created from state fish and wildlife licensing data for 1996 (if 1996 was

<sup>&</sup>lt;sup>24</sup> Although store-bought fish may also contain pollutants originating from TRI facilities, modeling this exposure pathway is not currently possible.

not available, 1997 was used). The number of fishing licenses in a county is then divided by the 1990 total population in the county.<sup>25</sup> The resulting ratio is multiplied by the population in each grid cell to obtain the number of individuals with fishing licenses within that cell. To account for family members who also eat fish caught by one member, the model multiplies the number of fishers by 2.62, the size of the average U.S. household in 1995 (U.S. Census Bureau, 1996). The total population in a grid cell consuming non-commercial fish is described by the following equation:

$$FishPop_{cell} = TotalPop_{cell} \bullet \frac{Licenses}{Pop} \bullet FamSize$$
(Eq. 5.20)

where:

FishPop <sub>cell</sub>	=	total fish-eating population in a grid cell,
$TotalPop_{cell}$	=	total resident population in a cell (see Section 5.1.3),
Licenses	=	number of fishing licenses in the county or state,
Pop	=	total population in the county or state in 1990, and
FamSize	=	average family size.

Next, the population that consumes fish is then apportioned based on whether fish are eaten recreationally or for subsistence. Recreational fishers may fish during only certain times of the year for recreational purposes or to supplement their diet. In contrast, subsistence fishers may fish throughout the year and a major part of their diets may consist of fish they catch. Data are lacking on numbers of recreational compared to subsistence fishers; RSEI follows guidance from EPA's Office of Water (Harrigan, 2000). The model assumes that of the population that eats non-commercial fish, 95 percent eat fish on a recreational basis, and the remaining 5 percent subsist on fish. This apportionment is described by the following relationships:

$$RecPop_{cell} = FishPop_{cell} \bullet 0.95$$
 (Eq. 5.21)

$$SubsistPop_{cell} = FishPop_{cell} \bullet 0.05$$
 (Eq. 5.22)

<sup>&</sup>lt;sup>25</sup> If no licensing information for a county was available, all of the grid cells in that county are assigned the ratio of total state licenses to total state population. If no information was available for the state in which the grid cell is located, ratio for the state closest to that grid cell is assigned.

where:

<i>RecPop</i> <sub>cell</sub>	=	recreational fishers (and families) in a cell, and
SubsistPop <sub>cell</sub>	=	subsistence fishers (and families) in a cell.

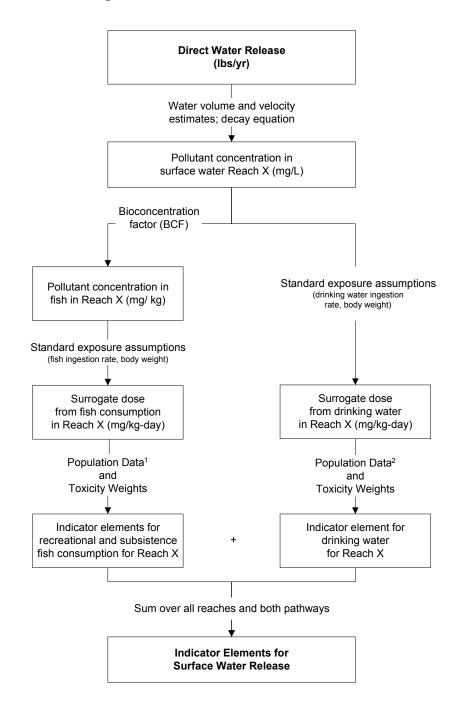
The fishing population in each cell is then assigned to specific stream reaches where they are presumed to catch fish. This is done in two steps. First, overlapping circles of 80-km radii associated with each of the two to seven points that describe individual stream reaches are used to define those grid cells that will be modeled for fishing population in the 48 contiguous states (i.e., all fishing areas within 80 km of all stream reaches). The distance of 80 kilometers (50 miles) from the reach is chosen based on a finding reported in the *1991 National Survey of Fishing, Hunting, and Wildlife-Associated Recreation* that 65 percent of anglers travel less than 50 miles to fish (U.S. Department of the Interior, 1993). This distance approximates the size of many counties and corresponds with the use of county-level fishing license data.

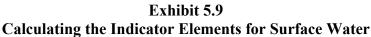
Second, all reaches within an 80-km radius of the center of each grid cell from the first selection are identified. The fish-eating population in the grid cell is apportioned to each surrounding stream reach based on the ratio of the length of that reach to the total reach kilometers within 80 km of the cell. For example, Reach A and B may be located within 80 km of a given cell. If Reach A is 15 km in length and Reach B is 5 km in length (and the entire length of each reach is completely within 80 km of the cell), then a total of 20 km of stream reaches are located within the specified distance. Because Reach A represents three-fourths (15/20) and Reach B represents one-fourth (5/20) of total km, the model therefore assumes that three-fourths of the fishing population in the cell catches fish from Reach A and one-fourth catches fish from Reach B. Note that the model uses only the portion of the reach's length that is within 80 km of the cell.

Because of the size of the database created, the fishing population data attributed to individual reaches is summed and stored at the reach level. The percentage of people in each of the ten agesex categories for the aggregated total fishing population (reflecting the ratio of the various age and gender subpopulations in the neighboring grid cells) is also maintained for each reach. The model then matches the chemical concentration in fish in the appropriate reach ( $C_{fish,reach}$ ) to the correctly-apportioned population. This is done for all reaches that have modeled chemical concentrations.

## 5.4.2 Calculating the Indicator Element for Surface Water

The Indicator Elements for drinking water and fish ingestion are calculated by generating for each unique combination of chemical release, stream reach, and exposure pathway a surrogate dose, then multiplying this dose by the toxicity weight of the chemical released and the estimated population. The RSEI risk-related result (score) for a surface water release from a TRI facility is calculated by adding the drinking water element and the fish consumption elements (recreational and subsistence fishing) for each reach and then summing over all reaches affected by the release (up to 200 km downstream from the facility). Exhibit 5.9 shows the approach for calculating the three Indicator Elements for surface water.





<sup>1</sup> Estimated using fish license data, household size, and distance traveled to fish
<sup>2</sup> Served by drinking water intakes in Reach X (if any)

Version 2.1 January 2004 1988-2000 TRI data

# 5.4.3 Surface Water Releases: Data

A variety of data are required to estimate exposure to chemical discharges to surface waters. The parameters required for surface water modeling and the data sources are described below and listed in Exhibit 5.10.

Parameter	Value (Units)	Source/Comment
Stream reach location	Lat/long in decimal degrees	RF1 (EPA, 1996)
Drinking water intake location and population served	Lat/long in decimal degrees Number of persons	SDWIS (2002)
Water flow	site-specific harmonic mean flow (million L /day)	calculated from RF1 (EPA, 1996)
Decay rate of chemical in water	chemical-specific (sec <sup>-1</sup> )	SRC (1994-99)
Chemical concentration in stream	(mg/L)	calculated
Bioconcentration factor	chemical-specific (L/kg)	SRC (1994-99); Lyman et al. (1990); EPA (1999)
Fish tissue concentration	calculated (mg/kg)	
Family size	2.62	U.S. Census Bureau (1996)

#### **Exhibit 5.10** Surface Water Modeling Parameters

#### 5.4.3.1 Stream reaches

Each facility is assumed to discharge into the nearest stream reach within six kilometers of the facility. If no reach is found within six kilometers, then the discharge is not modeled. The stream reaches used in the model are linear sections of streams, lakes, reservoirs, and estuaries that are linked to form a skeletal structure representing the branching patterns of surface water drainage systems. Non-transport reaches (i.e., those that do not have an upstream or downstream connection) are excluded from the model. The stream reach data are based on EPA's Reach File

Version 2.1 January 2004 Version 1.0 (RF1) for the conterminous United States. RF1 is a database that identifies and subdivides streams and shorelines of the United States to provide a hydrological framework for organizing water resource data. RF1 was prepared by the EPA in 1982 in support of the Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) system. RF1 consists of approximately 68,000 reach segments, comprising 700,000 miles of streams, and utilizes the Federal Information Processing Standards (FIPS) Hydrologic Unit drainage basin codes. This connectivity enables the Reach Files to provide both hydrologic ordering of stream locations using reach codes (i.e., what is upstream and downstream of a given point in the stream network can be readily determined) as well as network navigation proceeding in either the upstream or downstream direction. The metadata for the RF1 database can be found online at http://www.epa.gov/owowwtr1/monitoring/rf/rf1\_meta.html. RF1 does not contain data for Alaska, Hawaii, Puerto Rico, the U.S. Virgin Islands, Guam, American Samoa and the Northern Mariana Islands; therefore, RSEI does not model surface water releases for these areas.

The model uses stream reach attribute data from RF1 that describes water flow and velocity, as well as data that describe the reach location and the upstream and downstream reaches it connects to (these define the stream path for the chemical release). In RF1, 2,300 reaches in the Washington/Oregon area were identified as having no velocities despite having positive flow values. In these cases, information available in RF1 was used to calculate velocities for these reaches, using the following equation:

$$V = \frac{1.486}{Pmann} * Pdepth^{2/3} * Pslope^{1/2}$$
(Eq. 5.23)

where:

V	=	calculated stream velocity
Pmann	=	Mann's coefficient (from RF1)
Pdepth	=	depth of stream (from RF1)
Pslope	=	slope of stream (from RF1)

These calculated data allowed the creation of a complete data set for RF1 stream reaches. To this data set, certain criteria were applied to select the reaches to be used in the model. Specifically, because RSEI calculates the movement of a chemical release downstream using flow and velocity data, qualifying reaches must have at least one downstream or upstream connecting reach, and have a positive flow and velocity. Applying these criteria resulted in a final data set of 68,581 reaches for use in the model.

## 5.4.3.2 Drinking water intakes and populations

Drinking water intakes were obtained from EPA's Safe Drinking Water Information System (SDWIS) database.<sup>26</sup> SDWIS is a publically-accessible database that contains the information EPA uses to monitor public water systems. The database contains information on over 172,000 water systems, which serve over 90 percent of the U.S. population.<sup>27</sup> SDWIS is operated and maintained by EPA's Office of Water. There were approximately 7,300 records (each record describes a unique drinking water intake) in the original data set. From this set, records without necessary information (such as population) were deleted, leaving approximately 6,600 drinking water intakes.

Among these approximately 6,600 intakes, some intake records had no lat/long data, but did have valid county information. For each county with one of these intakes (approximately 600), all of the qualifying stream reaches were identified (see above for definition of qualifying reaches). The SDWIS populations associated with each drinking water intake were then divided evenly among the reaches (or the portions of the reaches) in the county where the intake is located; there is no apportionment based on the length of the reach. For instance, if there are two reaches in a county with one of these intakes, each reach is assigned half of the population for that intake. If more than one drinking water intake is located in a county, the distributed intake populations for each reach from each intake are summed for the individual reach(es). Exhibit 5.11 shows the number of intakes whose populations were distributed over more than one reach, by the state in which the intake is located.

State	Number of Intakes	State	Number of Intakes
AL	6	NV	28
AR	2	NY	2
AZ	5	OH	44
CA	75	OR	11
CO	9	SC	8

#### **Exhibit 5.11** State Location of Distributed Drinking Water Intakes

<sup>26</sup> Lee Kyle of EPA's Office of water provided a frozen data set (July 2002) for use in the model for RY 2000.

<sup>27</sup> Statistics are from EPA's Center for Environmental Information and Statistics (CEIS) review of SDWIS, based on 1996 data, on the internet at http://www.epa.gov/eq/ceisdocs/sdwis/sdwis-ex.htm .

State	Number of Intakes	State	Number of Intakes
IN	1	SD	3
KS	38	TN	2
KY	2	TX	19
LA	57	UT	1
MA	23	VA	2
ME	2	VT	74
MI	73	WA	9
МО	1	WI	14
MT	5	WV	4
NJ	17	WY	5
NM	19		
		Total	561

#### 5.4.3.3 Water flow

The RF1 stream flow data consist of estimates of mean annual flow and low flow (7Q10, the lowest flow over a seven day period to occur in ten years). These estimates were made at the downstream ends of more than 60,000 transport reaches and were coupled to an estimate of the time-of-travel velocity for the full length of those same reaches under each of the two flow regimes. RSEI uses the harmonic mean flow rate. The harmonic mean field in RF1 is not populated, so the harmonic mean is calculated from two other fields found in RF1: MNFLO, the mean annual flow at the base of the immediate reach, and SEVTEN, the 7-day-10 year low flow at the base of the immediate reach. The equation, taken from Chow (1959), is as follows:

$$HM = 1.194 * Mnflo^{0.473} * Sevten^{0.552}$$
 (Eq. 5.24)

where:

HM	=	harmonic mean flow (ft3/sec)
Mnflo	=	mean annual flow (ft3/sec)
Sevten	=	7-day-10 year low flow (ft3/sec)

Version 2.1 January 2004 1988-2000 TRI data

## 5.4.3.4 Water Decay Rates

Water decay rates are required to model downstream chemical concentrations. The primary sources for water decay values were Syracuse Research Corporation's (SRC's) ChemFate database, a component of SRC's Environmental Fate Data Base (SRC, 2002a), which contains experimental data, and SRC's Aqueous Hydrolysis Rate Program, HYDROWIN (part of the EPI suite of estimation programs (SRC, 1994-1999)), both of which were developed for the Environmental Protection Agency. The ChemFate database contains environmental fate and physical/chemical property information for commercially important chemical compounds, including TRI chemicals. HYDROWIN estimates hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkyl halides. Values of water decay rates can be found in Technical Appendix B.

#### 5.4.3.5 Bioconcentration Factors

Bioconcentration factor (BCF) is the term used to describe the equilibrium concentration of chemicals in aquatic organisms living in contaminated water. The BCF is defined as the ratio of the chemical concentration in the organism (mg/kg) to that in the surrounding water (mg/L). The term "bioconcentration" refers to the uptake and retention of a chemical by an aquatic organism *from the surrounding water only.*<sup>28</sup> Experimental BCF values were obtained from SRC's ChemFate database. Other BCFs were estimated from either log( $K_{ow}$ ) values using regression equations from Lyman et al. (1990), or from the SRC estimation program BCFWIN. See Technical Appendix B for values and references for the bioconcentration factors used in the model.

## 5.4.3.6 Human Exposure Assumptions

**Drinking Water.** For the drinking water pathway, the model uses estimates for the amount of tapwater ingested to estimate exposure. As in the stack and fugitive air pathways, data is acquired from EPA's Exposure Factors Handbook (EFH) (EPA, 1997b). EFH recommends mean tapwater intakes from two key studies, Ershow and Cantor (1989) and the Canadian Ministry of National Health and Welfare (1981) (as cited in EPA, 1997b, Table 3-30, p. 3-26). Because Ershow and Cantor (1989) provide body weight adjusted intakes, EFH recommends using this data in preference to data from the Canadian Ministry of National Health and Welfare (1981). As

<sup>&</sup>lt;sup>28</sup> The BCF can underestimate the accumulation of chemicals that are highly persistent and hydrophobic relative to the bioaccumulation factor (BAF), which measures the uptake and retention of a chemical by an aquatic organism *from all surrounding media (e.g. water, food, sediment)*. The bioaccumulation factor (BAF) is defined as the ratio of the chemical concentration in the organism (mg/kg) to that in the surrounding water (mg/L), in situations where both the organism and its food are exposed. Due to data limitations at the present time, only BCFs are used in the RSEI model.

a result, the RSEI exposure factors are based on data from Ershow and Cantor (1989). The age groups presented for the recommended values are, in some cases, broader than those used in RSEI. However, EFH also presents more refined age-specific intakes for the preferred study (Table 3-7, p.3-6). Drinking water intake rates per body weight were calculated for each of the modeled groups (male/female: ages 0-17, 18-44, 45-64, 65+)<sup>29</sup> using the weighted average approach presented in Equation 5.14. The final drinking water exposure factors are presented in Exhibit 5.12. Since body weight was already incorporated into the intake rates and sex-specific intake rates were not presented, the drinking water exposure factors are equivalent for males and females. More detail on the derivation of exposure factors can be found in Technical Appendix C.

Model Age Group	Exposure Factors (Male)	Exposure Factors (Female)
	(L/kg	g-day)
0-17	0.0298	0.0298
18-44	0.0184	0.0184
45-64	0.0220	0.0220
≥65	0.0219	0.0219

#### Exhibit 5.12 Drinking Water Exposure Factors

**Fish Ingestion.** RSEI uses annual estimates of the amount of fish ingested by recreational and subsistence fishers and their families. However, there are no national data on fish ingestion rates specific to recreational and subsistence fishers. In the absence of such data, RSEI uses fish ingestion rates from the 1994-1996 USDA Continuing Survey of Food Intake by Individuals (CSFII). This survey was conducted by the U.S. Department of Agriculture in 50 states and the District of Columbia over a three-year period. A total of 15,303 individuals provided two non-consecutive days of data on dietary intake. Appropriate statistical techniques were used to extrapolate to the national population. In a 2000 publication, EPA assigned specific fish species to habitats (freshwater, estuarine, and marine) based on the majority of time the species spend in

<sup>&</sup>lt;sup>29</sup> The RSEI model provides the ability to view risk scores for the 0-9 year old age group, however, there is not a separate exposure factor for this age group. Instead, the exposure factor for the 0-17 year old age group is used.

those habitats (EPA, 2000). Based on these assignments, EPA estimated a distribution of uncooked finfish and shellfish ingestion rates specific to freshwater and estuarine fish.<sup>30</sup> As recommended by EPA's Office of Water (Tudor et al., 2000), for environmental assessments the 90<sup>th</sup> percentile is used to represent ingestion rates for recreational fishers, and the 99<sup>th</sup> percentile is used for subsistence fishers. The ingestion rates are reported by age group (<15 years, 15-44 years, 45+ years) and sex (EPA, 2000). These values are roughly similar to ingestion rates obtained from regional studies of recreational fishers and subsistence fishers, respectively. Fish ingestion values were estimated for the RSEI age groups using Equation 5.15. These values are then divided by age- and sex-specific body weights, averaged to match the RSEI age groups using data provided in EFH (EPA, 1997b, Tables 7-2 and 7-3, p. 7-4). Exhibit 5.13 presents the fish ingestion rates used in the model. More detail on the derivation of exposure factors can be found in Technical Appendix C.

Exhibit 5.13
Fish Ingestion Exposure Factors

	Recreational (g/kg-day)*		Subsistence (g/kg-day)*	
Model Age Group	Male	Female	Male	Female
0-17	0.0756	0.0372	2.83	2.05
18-44	0.199	0.114	1.92	1.71
45-64	0.407	0.262	2.08	1.60
≥65	0.434	0.267	2.22	1.63

\* Fish ingestion exposure factors are converted to kg/kg-day for the surrogate dose calculation in the model.

<sup>&</sup>lt;sup>30</sup> Consumption of marine fish is not included in the ingestion rates, because marine areas are not modeled in RSEI.

# 5.5 Modeling Transfers to POTWs

In 2000, approximately three percent of TRI emissions were transferred to Publicly-Owned Treatment Works (POTWs). These transfers are mostly of facility wastewater through underground sewage pipes to a POTW. Each chemical transfer to a POTW is modeled as entering as liquid influent. Depending on the chemical's physical properties, some portion of the chemical release in the influent may be discharged into surface water from the POTW, potentially resulting in human exposure through drinking water or fish ingestion. The rest of the chemical release may be removed by the POTW through one or more of the following processes: 1) biodegradation, which is not modeled; 2) volatilization, which is modeled like other area air releases (see Section 5.2.3); or 3) landfilling of sludge, which is not modeled. The following sections describe the method and data used to model transfers to POTWs.

#### 5.5.1 Transfers to POTWs: Method

Modeling exposure from TRI-reported transfers to POTWs requires: (1) location of the POTW to which the chemicals are discharged, (2) location of the reach to which the POTW discharges, (3) consideration of overall removal efficiencies of POTWs and resulting effluent discharges from POTWs (the chemical-specific removal rate), and (4) consideration of residuals management at POTWs (partitioning within the POTW).

#### 5.5.1.1 Locating the POTW

In order to model releases from POTWs, these facilities must first be located on the model grid. Like other off-site facilities, POTW names and addresses are reported to TRI by the facility transferring its waste. Latitude and longitude are not reported. In order to derive lat/long coordinates, the reported street addresses were geocoded (coordinates were assigned based on street address).<sup>31</sup> Where possible, duplicate entries for the same POTW (in the common instance where two or more reporting facilities have transferred to the same POTW) were collapsed to a single entry using an approximate string matching program (see Technical Appendix D for details). Once latitude and longitude for a facility are determined, the data are used to map the facility to the grid cell with the same coordinates. Substantial data processing was necessary to prepare the data set of off-site facilities for use in the model; see Technical Appendix D for details on the steps that were taken.

<sup>&</sup>lt;sup>31</sup> Geocoding services were provided by Thomas Computing Services, a commercial firm.

## 5.5.1.2 Locating the POTW Discharge Reach

As with TRI reporting facilities, the POTW's discharge reach must be identified. Unlike other facilities in the model which are assumed to discharge to the nearest reach, EPA has information for the reaches to which POTWs discharge their wastewater. EPA's Permit Compliance System (PCS) <sup>32</sup> identifies the specific discharge reach for each POTW, as reported by the POTW itself. PCS contains National Pollutant Discharge Elimination System (NPDES) data, including permits, monitoring data, and locational and descriptive information pertaining to more than 67,000 facilities regulated under NPDES.<sup>33</sup> As there are no identifiers common to the TRI database and the PCS database, the approximate matching program described earlier was used to match the two sets of names and addresses. Approximately 3,000 POTWs were matched to a discharge reach using this method.

In addition, the 150 POTWs with the highest risk-related surface water score for RY 1998 were searched for individually in PCS. The high scores attributed to these facilities required some verification that the discharge reach being used in the model was correct. Of these 150 POTWs, slightly more than half were matched to a reach in PCS. In these cases, the discharge reach identified in PCS was used for the POTW. The remaining POTWs are assumed to discharge to the nearest reach.

#### 5.5.1.3 Overall POTW Removal Rate

POTWs cannot completely remove all of the chemicals that are transferred to the plant from the TRI facility. Some of the chemical loading in the influent will be discharged as effluent to surface waters. To calculate the fraction of transferred chemical removed by the POTW, the typical chemical-specific removal rate is applied to the volume transferred to the POTW from the TRI facility. See Technical Appendix B for the a listing of removal rates and references for each chemical. The remainder is assumed to exit the POTW in water effluent. This effluent is modeled for drinking water and fish ingestion using the same methods for surface water releases described above.

<sup>&</sup>lt;sup>32</sup> The following additional information was used in addition to PCS: the Industrial Facilities Discharge File (IFD), the NEEDS Survey, TRI, and the OPPT Task 73 Report. Where stream name but not reach number was available, USGS maps were used to manually assign reach numbers to named reaches.

<sup>&</sup>lt;sup>33</sup> EPA's Center for Environmental Information and Statistics (CEIS) provides an overview of PCS data at http://www.epa.gov/ceisweb1/ceishome/ceisdocs/pcs/pcs-exec.htm.

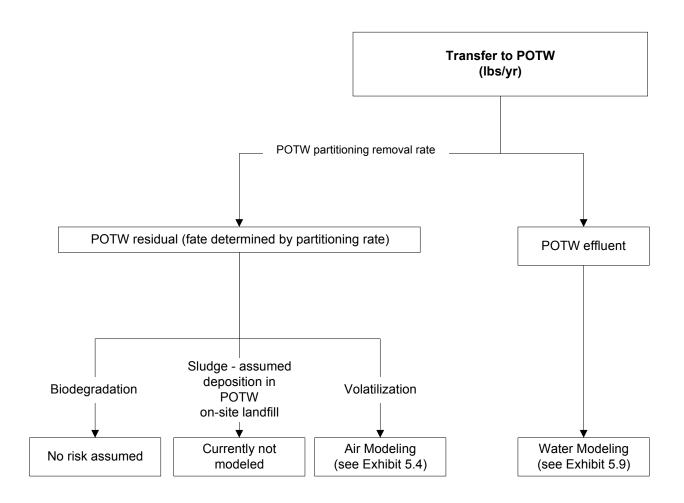
## 5.5.1.4 Partitioning within the POTW

Chemical loadings may be removed by the POTW treatment processes through biodegradation, volatilization, and adsorption to sludge. The amount of the chemical that is removed by each of these processes is modeled using average partitioning rates (see Technical Appendix B for the listing of partitioning rates and references for each chemical).

Once the fates of chemicals entering the POTW are estimated, exposures associated with chemical loadings to each compartment are estimated. Chemicals discharged in the POTW effluent are modeled using the surface water evaluation methods described above. Chemicals that biodegrade are assumed to degrade to chemicals that do not pose risk. POTW volatilization releases are treated like area-source air releases, as described earlier.

For chemicals that partition to sludge, the model used to estimate exposure should ideally depend on the sludge disposal method employed by the POTW. However, sludge disposal practices at a POTW receiving a TRI transfer cannot be determined from the TRI database. Therefore, the model algorithm currently assumes all POTW sludge is landfilled at the POTW, a common method of sludge disposal. POTWs may in reality use other methods of sludge disposal, such as incineration of sludge. If sludge were incinerated by a POTW, for example, this would result in different exposure levels (and a different, larger exposed population). RSEI does not currently model land releases. A summary of the approach to modeling POTW emissions is found in Exhibit 5.14.

Exhibit 5.14 POTW Modeling Approach



## 5.5.1.5 Estimating Population Size for POTW Transfers

The population exposed to air releases is assumed to be the population within a 101-km by 101-km grid around the POTW. The method used to estimate the population surrounding the POTW that is exposed to surface water effluent discharges up to 200 km downstream from these facilities is described in the section on exposed populations for surface water releases (see Sections 5.4.1.2 and 5.4.1.4.)

# 5.5.2 Transfers to POTWs: Data

Exhibit 5.15 presents data used to estimate exposure from releases to POTWs. In addition to the parameter data presented here, data from the air release pathway (see Exhibit 5.5), and water release pathway (see Exhibit 5.10) are also used. Environmental fate and transport data and exposure factors specific to these pathways are described in the relevant sections above.

Parameter	Value	Source/Comment	
Removal efficiencies	chemical-specific	RREL or STPWIN (SRC, 1994-99)	
Partitioning within the POTW	chemical-specific	RREL or STPWIN (SRC, 1994-99)	

**Exhibit 5.15.** Data Used to Estimate Exposure from Releases to POTWs

#### 5.5.2.1 POTW Removal Rate Efficiency and Within-POTW Partitioning

Data specific to this pathway include POTW removal efficiencies and within-POTW partitioning rates. These parameters describe the fate of chemicals during treatment at POTWs. The "POTW Partition Removal" is the total POTW removal efficiency, or the total percentage of the chemical removed by the POTW (influent minus effluent). The within-POTW partition values describe the fate of that portion of the chemical removed, that is, whether the chemical may sorb to sludge (POTW Partition Sludge), volatilize into the air (POTW Partition Volatile) or be biodegraded by microorganisms (POTW Partition Biodeg). The within-POTW partitioning values are expressed as percentages of the total POTW removal efficiency; that is, they sum to 100 percent.

POTW removal efficiencies were obtained from the Treatability Database maintained by the EPA Risk Reduction Engineering Laboratory (RREL). For any given chemical, the RREL Treatability Database provides a list of removal efficiencies published in the scientific literature. Each value is characterized by the technology used, the type of influent, and the scale of the experiment. For all values associated with activated sediment and full scale experiments, a geometric mean was derived and used as the POTW removal efficiency. Within-POTW partitioning values were obtained from two sources. For most organic chemicals, values were supplied by the EPA's Exposure Assessment Branch within OPPT. Inorganic chemicals, except for ammonia, were assumed to partition 100% to sludge. For chemicals without data from these sources, SRC's Sewage Treatment Plant Fugacity Model (STPWIN) was used to estimate total removal efficiency and within-POTW partitioning values.

# 5.6 Modeling Other Off-site Transfers

In 2000, approximately 35 percent of TRI emissions were transferred to off-site locations for storage or disposal. TRI reporters are required to supply the name and address of the receiving facility, and the treatment method used. Currently, only transfers that are incinerated at the off-site facility are modeled; waste transfers treated by other methods do not receive risk-related scores.

## 5.6.1 Off-site Transfers: Method

To assess the exposure potential associated with off-site transfers, it is important to have information about the off-site facility location and some of its characteristics. Locations of other off-site facilities are determined in the same way as the locations of POTWs: all of the off-site facilities were geocoded based on their street address and zip code, and then duplicate entries for the same off-site facility were removed. The remaining off-site facilities were mapped to the grid based on their assigned coordinates. See Technical Appendix D for detailed information on locating off-site facilities.

The TRI forms require the reporting facility to indicate the treatment/disposal method used at the off-site facility. If this information is not reported (despite the requirement), the transfer is not evaluated in the algorithm, but is flagged as a missing value and assigned a zero.

If the treatment method is incineration, then destruction and removal efficiencies (DREs) are applied to the transfer amount. Once DREs have been applied, the releases are modeled using the ISCLT-based air modeling algorithms described earlier.

For off-site landfills, there are two exposure pathways, groundwater and volatilization. However, as land releases are not currently modeled, there are no risk-related results available for either pathway. Off-site transfers to underground injection wells are also not modeled. Exhibit 5.16 summarizes the modeling of off-site transfers.

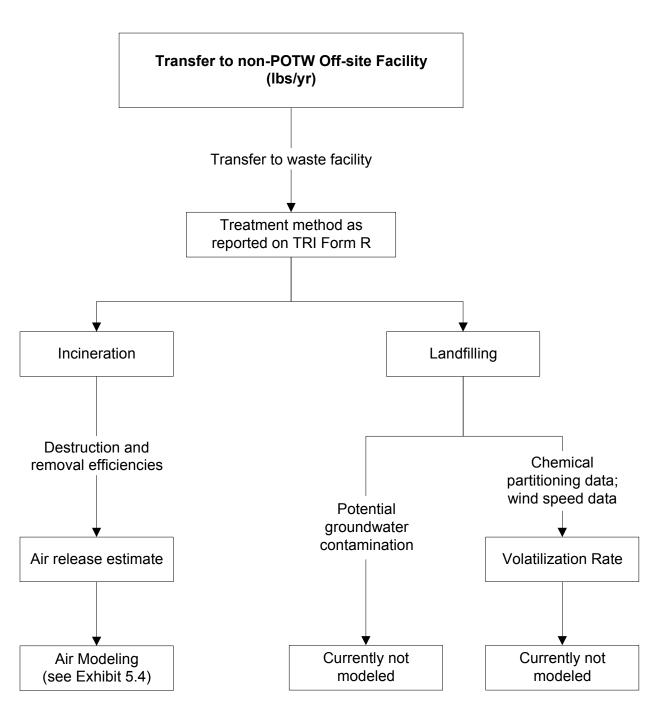


Exhibit 5.16 Modeling Approach for Off-site Transfers

Version 2.1 January 2004 1988-2000 TRI data

#### 5.6.2 Estimating Population for Off-Site Transfers

Similar to on-site air releases, the population exposed to air releases from off-site transfers is the population within a 101-km by 101-km grid around the off-site incinerator.

#### 5.6.3 Off-site Transfers: Data

#### 5.6.3.1 Destruction and Removal Efficiencies

For organics, the destruction and removal efficiency (DRE) is assumed to be 99 percent (see Technical Appendix B). The exception to the 99 percent removal assumption are PCBs, which are assumed to have a DRE of 99.9999 percent, as required by TSCA regulation. For inorganics, values are taken from multiple hearth sludge incinerator studies (EPA, 1992a).

# 5.7 Modeling On-site Land Releases

In 2000, approximately 41 percent of TRI emissions were released as on-site land releases. Onsite land releases include releases to landfills, surface impoundments, land treatment units, and underground injection wells. For these releases, two major exposure pathways are of interest volatilization to air and leaching into groundwater. Volatilization of chemicals from on-site land releases is reported to TRI under the fugitive emission estimate for the facility, and is modeled by RSEI as part of the facility's fugitive air release. For more information on RSEI modeling of fugitive air releases, see Section 5.3 above. EPA is evaluating screening-level methodologies which might be used to assess risk-related exposures pertaining to groundwater exposure from on- and off-site land releases and volatilization from off-site land releases, so this version of RSEI does not provide risk modeling for reported land releases. However, RSEI does provide the capability for users to examine the pounds of releases to land that are reported to TRI, as well as viewing these releases from a hazard-based perspective.

The potential for groundwater contamination from land releases depends on the regulatory status of the unit in which the chemical is released. For example, chemicals could be deposited in an on-site RCRA-regulated, subtitle C 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, EPA assumes that releases to groundwater are negligible so RSEI assigns a zero value to the risk-related scores for such releases. If chemicals are placed in nonhazardous land disposal units (landfills, etc.), there is a potential for exposure. This exposure pathway and volatilization from off-site landfills are currently under review for inclusion in a future version of RSEI.

On- and off-site land releases to underground injection will not be modeled for exposure by RSEI. The hydrogeological, spatial, and temporal considerations that are associated with exposures to toxic chemicals in underground injection wells are situation- and site-specific, so RSEI is only able to provide pounds-based and hazard-based perspectives for this type of land release. Note, however, that under well-managed conditions, Class I wells (there are five classes of wells) are specifically designed to pose minimal risk to human health or the environment.

# 6. Calculating Results

This section summarizes the computation of the principal types of RSEI results. Because of the multi-functional nature of the model, a wide variety of results can be created. All of the RSEI functionality is based upon the Indicator Element, which is a unique combination of chemical, facility, release and exposure pathway, and year. Each Indicator Element has a set of associated results:

Exhibit 6.1 Description of RSEI Results

Risk-related results	Surrogate Dose <b>x</b> Toxicity Weight <b>x</b> Population	
Hazard-based results	Pounds <b>x</b> Toxicity Weight	
Pounds-based results	TRI Pounds released	

**Risk-related results.** The surrogate dose, toxicity, and population components are multiplied to obtain a risk-related score for the Indicator Element. The surrogate dose is determined through pathway-specific modeling of the fate and transport of the chemical through the environment, combined with subpopulation-specific exposure factors. Risk-related scores are unitless, and each of the components (toxicity weight, surrogate dose, and population) when multiplied provide scores that are relevant only when compared to each other. The unitless Indicator Elements are not a physically meaningful measure of quantitative risk associated with the facility, but are approximate measures of relative risk-related impacts that are comparable to approximate measures for other facilities (or other chemicals, pathways, etc.) calculated using the same methods within RSEI. If the Indicator Element cannot be modeled, because of a lack of data required for modeling, or because the pathway is not currently modeled, then the risk-related score is zero. The model calculates risk-related results for the entire population and also for the following subpopulations: children under 10, children aged 10 to 17, males aged 18 to 44, females aged 18 to 44, and adults aged 65 and older. In addition the model also calculates "Modeled Pounds," which is simply the number of pounds that can be modeled, before fate and transport modeling and exposure assumptions have been applied.

Higher component "weights" are associated with higher relative risk-related values (and lower weights are associated with lower relative risks). For chemicals with cancer effects, multiplying the weights associated with cancer toxicity and exposure to the chemical seems intuitive, since this is similar to the calculation of cancer risk with a slope factor or unit risk value and dose or exposure level. For chemicals with noncancer effects, the multiplicative nature of the toxicity and exposure weights may not seem intuitive, because in risk assessments, risk is usually characterized as the estimated exposure divided by the RfD/RfC. However, because of the

Version 2.1 January 2004 manner in which the toxicity weights have been constructed, the product of toxicity weight and surrogate dose varies in the same direction and degree as the ratio of exposure to RfD/RfC. This is because the toxicity weight is inversely related to the magnitude of the RfD/RfC. Thus, for a given exposure level, a chemical with a more stringent (i.e., lower) RfD will receive a higher Indicator Element value than a chemical with a less stringent (i.e., higher) RfD, as shown in the following example:

	RfD (mg/kg- day)	Toxicity Weight	Surrogate dose (mg/kg- day)	Exposure (i.e., surrogate dose) /RfD Ratio	Toxicity Weight * Surrogate Dose
Scenario 1	0.1	5	1	1/0.1 = 10	5*1 = 5
Scenario 2	0.01	50	1	1/0.01 = 100	50*1 =50

**Exhibit 6.2 Example of Scoring for Noncancer Effect** 

Since no adverse effects are expected to occur below the RfD, one could argue that releases that result in surrogate doses below the RfD should be excluded. However, this approach was not pursued for the following reasons: first, the estimation of surrogate dose is only a screening-level approximation for the purposes of comparing one release to another in a relative way, and should never be considered an actual calculation of exposure. To exclude releases resulting in surrogate doses below the RfD would incorrectly imply that the method could predict precisely when doses would occur below the RfD. Second, exposure to the same chemical from multiple facilities, or multiple chemicals from one or more facilities affecting the same health endpoint could act additively to pose risk, even if each release individually did not exceed the RfD. Finally, if the surrogate dose is low, this will be reflected by a correspondingly low score relative to other releases for that chemical.

**Hazard-based results.** Each Indicator Element also is associated with a hazard-based result ("Hazard"), calculated by multiplying the pounds released by the appropriate chemical-specific toxicity weight (the toxicity weight also depends on the exposure pathway). The inhalation toxicity weight is used for releases or transfers to fugitive air, stack air, off-site incineration, and off-site incineration-no fuel value. The oral toxicity weight is used for releases or transfers to direct water and POTWs. For releases that are not modeled (because the pathway is not modeled or because other necessary data, such as physicochemical properties, are lacking), the higher toxicity weight is used. For these results, no exposure modeling or population estimates are

involved. If there is no toxicity weight available for the chemical, then the hazard score is zero.

The model also calculates "Modeled Hazard," which is the chemical- and pathway-specific toxicity weights multiplied by the Modeled Pounds (as described above), and "Modeled Hazard \* Pop," which multiplies modeled hazard by the potentially exposed population, but without the fate and transport modeling (and application of exposure assumptions) that would be found in risk-related results.

**Pounds-based results.** These results ("TRI Pounds") reflect only the number of pounds released or transferred that are reported to TRI, and are available for virtually all Indicator Elements. The model also provides "TRI Pounds with Toxicity Weights," which simply sums the pounds for chemicals that have toxicity weights in RSEI.

## 6.1 Combining Indicator Elements

Once results are calculated for each Indicator Element, they can be combined in many different ways. All of the results are additive, so a result for a specific set of variables is calculated by summing all the relevant individual Indicator Element results, as follows:

$$R = \sum \sum \sum IE_{c,f,p}$$
(Eq. 6.1)

where:

R = RSEI result, and  $IE_{c,f,p} =$  chemical-facility-pathway-specific Indicator Element result.

This method is very flexible, allowing for countless variation in the creation of results. For example, results can be calculated for various subsets of variables (e.g., chemical, facility, pathway) and compared to each other to assess the relative contribution of each subset to the total potential impact. Or, results for the same subset of variables for different years can be calculated, to assess the general trend in pounds-based, hazard-based, or risk-related impact over time.

It must be reiterated that while changes in results over the years would imply that there have been changes in hazard- or risk-related environmental impacts, the actual magnitude of any specific change or the reason may not be obvious. Although the value itself may be useful in identifying facilities or chemicals with the highest potential for hazard or risk, the score does not represent a quantitative estimate or provide an exact indication of the magnitude of individual hazard or risk associated with that facility or chemical.

## 6.2 Accounting for Changes in TRI Reporting

When a change occurs in the number of, or reporting requirements for, chemicals and facilities represented in TRI, the numerical value of RSEI results will be altered if no adjustments are made to the method of calculation to account for the changes respective to trend analyses. However, such changes would not necessarily represent a large change in actual environmental impact, but would reflect a broader understanding of the impacts that may have always existed.

A change in the number of chemicals and facilities in the TRI can occur through several mechanisms. First, the addition to or deletion of individual chemicals from the TRI chemical list will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. Several additions and deletions to the data set have already occurred since 1987 (the first year of TRI reporting). Furthermore, the Agency added 245 chemicals and chemical categories to the TRI chemical list in a single year, effective in 1995. The deletion of chemicals would presumably have a minor effect since such chemicals would be deleted due to their low hazard. Delisted chemicals are removed from RSEI. To account for changes in the representation of chemicals in the TRI database, RSEI uses a special identifier called "Core Chemical" which denotes chemicals that have been listed on the TRI since the first year (1987) of reporting and which have had no change in their reporting requirements. Another identifier, "Mini Core" denotes chemicals that have been listed on the TRI since 1995 and which have had no change in their reporting requirements. These identifiers allow users to conduct separate analyses for the "Core" or "Mini Core" chemicals, and so exclude chemicals whose emissions changes over time are caused by reporting requirement changes. Similarly, the 245 chemicals added for the 1995 reporting year can also be analyzed separately.

Facility-level changes can also affect year-to-year scores generated using RSEI. For instance, compliance with TRI reporting has improved over time, which has led to more facilities reporting. Increases in the number of reporting facilities may occur as a result of changes in reporting requirements. For instance, in the first two years of reporting, facilities that manufactured or processed more than 50,000 pounds were required to report their releases. However, EPCRA lowered this threshold to 25,000 pounds in 1989. For reporting year 2000, thresholds and other reporting requirements for 18 Persistent Bioaccumulative Chemicals (PBTs) have been changed. These modifications can act to alter the total emissions reported to the TRI and the model's estimates of associated hazard- and relative risk-based impacts. Also, effective in the 1998 reporting year, certain SIC codes were added to TRI, adding to the universe of

reporting facilities.<sup>34</sup> To assist users in separating out the effects of the 1998 expansion, RSEI allows for the exclusion of facilities in the newly-required SIC codes when doing trend analyses.

The yearly TRI reporting data for a given list of chemicals and facilities are the subject of ongoing quality control review and revision. As a result, yearly comparisons could be flawed if ongoing revisions by individual facilities were not included in each year's results. Therefore, the Indicator Elements are re-computed for all years in the database on an annual basis in order to incorporate revisions to the reporting data. This annual calculation is based on the corrections incorporated in annual Public Data Releases available from EPA's TRI program.

<sup>&</sup>lt;sup>34</sup> This facility expansion rule required the affected facilities to report their releases for the 1998 reporting year. The added SIC codes are: codes 10 (except 1011, 1081, and 1094), 12 (except 1241), industry codes 4911, 4931 and 4939 (limited to facilities that combust coal and/or oil for the purpose of generating power for distribution in commerce), 4953 (limited to facilities regulated under RCRA), 5169, 5171, and 7389 (limited to facilities engaged primarily in solvent recovery services on a contract or fee basis) (EPA 1997a).

# 7. Current Implementation of the RSEI Method

# 7.1 RSEI Chronic Human Health Model

The RSEI method is a stand-alone program for the personal computer. The program allows users to calculate RSEI results for all years of data (1988-2000 reporting data) and to present the results in various GIS, graphical, and tabular formats, as well as to save selected data to other spreadsheet and database formats (e.g., Microsoft Excel and databases such as Microsoft Access). The program includes on-line help for all of the program functions, as well as an introductory, "Easy RSEI" interface that simplifies first-time use. A User's Manual is also available for RSEI Version 2.1.

Users of the model can perform, in a matter of minutes or hours, a variety of screening-level analyses. Previously, such activities would have taken days, weeks, or even months to organize the relevant information, evaluate that information, and perform the complex and sophisticated analyses that are necessary to provide a risk-related perspective. Results can be used for screening-level ranking and prioritization for strategic planning purposes, risk-related targeting, and trends analyses. Considerable resources can be saved by conducting preliminary analyses with the model to identify risk-related situations of high potential concern, and which warrant further evaluation.

As noted above, users can evaluate releases using a number of variables, such as chemical, medium, geographic area or industry sector. For instance, the following types of questions can be investigated: How do industry sectors compare to one another from a risk-related perspective? What is the relative contribution of chemicals within a given industry sector? What release pathway for a particular chemical poses the greatest risk-related impacts? Users can view various pounds- and hazard-based results to investigate the relative influence of toxicity and population components on the risk-related results. However, only the risk-related results incorporate exposure modeling.

The model also contains fully integrated geographic capabilities. Users can select and display on maps the location of facilities and defined geographic areas, such as tribal lands. For a 101-kilometer square around a facility, the model will quickly and easily display grid-cell concentrations for chemical releases to air, and can sum the overlapping release plumes. In addition, for any small geographic area, users can display the population distribution for any population subgroup, and show the population-weighted air concentrations by subgroup. The currently released version of RSEI has full modeling of the air and surface water exposure pathways only, but future versions may provide full modeling of all exposure pathways.

Users should note that, as implemented for the personal computer, RSEI employs a facility-based approach. All modeled impacts are attributed to the facility originally releasing or transferring the chemical. For instance, an air release from an off-site incinerator is modeled as exposing the

population around the off-site facility, but the results (pounds, hazard, score, etc.) are attributed to the reporting facility that transferred the chemical to the off-site incinerator. Similarly, while impacts may extend beyond geographic boundaries such as zip code, county, or state, the results are attributed to the geographic entity in which the facility is located. EPA employs the RSEI methodology to create other databases which are geographic-based. These very large datasets are operated outside of the user-friendly interface provided by the RSEI model.

RSEI Version 2.1 is available without charge from EPA on an installation CD-ROM (EPA No. 774-C-02-001, December 2002). The installed RSEI model requires approximately 2 GB of hard disk space. It is designed for operation using a 32-bit operating system (Windows 95, 98, 2000, XP, and NT4). The program is written using Borland's Delphi (the software is coded in Object Pascal) and uses the Paradox file format. Information regarding the RSEI project is available on the RSEI web site.<sup>35</sup>

# 7.2 Conclusion

As an indication of improvements in environmental quality over time, RSEI provides EPA and the public with a valuable tool to measure general trends based upon the relative risk-related impacts of TRI chemicals. Although RSEI results do not capture all environmental releases of concern, they generally relate changes in releases to relative changes in chronic human health impacts from a large number of toxic chemicals of concern to the Agency. Importantly, RSEI provides an ability to analyze the relative contribution of chemicals and industrial sectors to human health impacts, and RSEI results serve as an analytical basis for setting priorities for pollution prevention, regulatory initiatives, enforcement targeting and chemical testing requirements.

<sup>&</sup>lt;sup>35</sup> For current information or inquiries regarding the Risk-Screening Environmental Indicators Project, please contact: Gary Cole, Ph.D., (202) 564-8808, cole.gary@epa.gov, or Cody Rice, (202) 564-8769, rice.cody@epa.gov. Or, see www.epa.gov/oppt/rsei.

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#### **RSEI** supporting documentation released by EPA

— these documents can be found on the RSEI website (under the Documents and Documents Archive headings) at http://www.epa.gov/oppt/rsei/documents.html.

User's Manual for RSEI Version 2.1. December 2002.

RSEI Version 2.1 FACT Sheet. January 2004.

RSEI Technical Appendices:

Technical Appendix A -	Listing of All Toxicity Weights for TRI Chemicals and Chemical Categories
Technical Appendix B -	Physicochemical Properties for TRI Chemicals and Chemical Categories
Technical Appendix C -	Derivation of Model Exposure Parameters
Technical Appendix D -	Locational Data for TRI Reporting Facilities and Off-site Facilities
Technical Appendix E -	Derivation of Stack Parameter Data
Technical Appendix F -	Summary of Differences Between RSEI Data and the TRI Public Data Release

- TRI Relative Risk-based Environmental Indicators: Summary of Comments Received on the Draft 1992 Methodology and Responses to Comments. Prepared for the Office of Pollution Prevention and Toxics, Economics, Exposure and Technology Division, Regulatory Impacts Branch. May 1997. Prepared by Abt Associates under Contract # 68-D2-0175.
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- Ground-Truthing of the Air Pathway Component of OPPT's Risk-Screening Environmental Indicators Model. December 1998.
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Version 2.1 January 2004 1988-2000 TRI data