**OAK RIDGE
NATIONAL
LABORATORY**

LOCKHEED MARTIN

RECEIVED

APR 01 1999

OST

**The Risk Assessment
Information System**

S. B. Kerr
R. R. Bonczek
C. W. McGinn
M. L. Land
L. D. Bloom
B. E. Sample
F. G. Dolislager

MASTER

MANAGED AND OPERATED BY
LOCKHEED MARTIN ENERGY RESEARCH CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

HH

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831; prices available from (615) 576-8401.

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

**Portions of this document may be illegible
electronic image products. Images are
produced from the best available original
document.**

THE RISK ASSESSMENT INFORMATION SYSTEM

S. B. Kerr
R. R. Bonczek
C. W. McGinn
M. L. Land
L. D. Bloom
B. E. Sample
F. G. Dolislager

June 1998

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *HH*

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831-6285
managed by
LOCKHEED MARTIN ENERGY RESEARCH CORP.
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-96OR22464

CONTENTS

	Page
ACKNOWLEDGMENTS	<u>v</u>
EXECUTIVE SUMMARY	<u>vii</u>
1. RISK ASSESSMENT INFORMATION SYSTEM OVERVIEW	<u>1</u>
2. PRELIMINARY REMEDIATION GOALS	<u>1</u>
2.1 AGRICULTURAL LAND USE	<u>2</u>
2.2 RESIDENTIAL LAND USE	<u>4</u>
2.3 INDUSTRIAL LAND USE	<u>4</u>
2.4 EXCAVATION LAND USE	<u>5</u>
2.5 RECREATIONAL LAND USE	<u>5</u>
3. REGULATORY LIMITS	<u>6</u>
4. TOXICITY AND CHEMICAL FACTORS	<u>7</u>
4.1 TOXICITY PROFILES	<u>7</u>
4.2 TOXICITY VALUES	<u>8</u>
4.2.1 NONRADIONUCLIDE CHEMICAL INFORMATION	<u>8</u>
4.2.2 RADIONUCLIDE INFORMATION	<u>9</u>
4.3 CHEMICAL-SPECIFIC FACTORS	<u>10</u>
5. HUMAN HEALTH RISK EXPOSURE MODELS	<u>11</u>
6. ECOLOGICAL BENCHMARKS	<u>11</u>
7. RISK RESULTS	<u>12</u>
8. OTHER INFORMATION	<u>13</u>
9. REFERENCES	<u>13</u>

ACKNOWLEDGMENTS

The authors would like to thank the staff of the Oak Ridge National Laboratory Toxicology and Risk Analysis Section of the Life Sciences Division for assistance in developing the Risk Assessment Information System. The authors would also like to thank T. C. Perry, T. L. Mims, and P. R. Siebach of the Department of Energy for their continued support and involvement in developing the Risk Assessment Information System.

EXECUTIVE SUMMARY

In an effort to provide service-oriented environmental risk assessment expertise, the Department of Energy (DOE) Center for Risk Excellence (CRE) and DOE Oak Ridge Operations Office (ORO) are sponsoring Oak Ridge National Laboratory (ORNL) to develop a web-based system for disseminating risk tools and information to its users. This system, the Risk Assessment Information System (RAIS), was initially developed to support the site-specific needs of the DOE-ORO Environmental Restoration Risk Assessment Program. With support from the CRE, the system is currently being expanded to benefit all DOE risk information users and can be tailored to meet site-specific needs. Taking advantage of searchable and executable databases, menu-driven queries, and data downloads, using the latest World Wide Web technologies, the RAIS offers essential tools that are used in the risk assessment process or anywhere from project scoping to implementation. The RAIS tools can be located directly at http://risk.lsd.ornl.gov/homepage/rap_tool.htm or through the CRE's homepage at <http://www.doe.gov/riskcenter/home.html>.

1. RISK ASSESSMENT INFORMATION SYSTEM OVERVIEW

To provide service-oriented environmental risk assessment expertise, Oak Ridge National Laboratory (ORNL) is developing a system of risk analysis tools and information resources for the World Wide Web (WWW). This work is sponsored by the Department of Energy (DOE) Center for Risk Excellence (CRE) and DOE Oak Ridge Operations Office (ORO). This system, the Risk Assessment Information System (RAIS), was initially developed to support the site-specific needs of the DOE-ORO Environmental Restoration Risk Assessment Program. With support from the CRE, the system is being expanded to benefit all DOE risk information users. Taking advantage of searchable and executable databases, menu-driven queries, and data downloads, using the latest WWW technologies, the RAIS offers essential tools that are used in the risk assessment process or anywhere from project scoping to implementation and can be tailored to meet site-specific needs. The RAIS tools can be located directly at http://risk.lsd.ornl.gov/homepage/rap_tool.htm or through the CRE's homepage at <http://www.doe.gov/riskcenter/home.html>. The following material discusses, the RAIS tools and information resources. These are: 1) Preliminary Remediation Goals (PRGs), 2) Regulatory Limits, 3) Toxicity and Chemical Factors, 4) Human Health Risk Exposure Models, 5) Ecological Benchmarks, 6) Risk Results and 7) Other Information.

2. PRELIMINARY REMEDIATION GOALS

As discussed in *Risk Assessment Guidance for Superfund, Volume 1, Human Health Evaluation Manual (Part B, Development of Risk-based Preliminary Remediation Goals)* (RAGS, Part B)(EPA 1991), chemical-specific PRGs are concentration goals for individual chemicals in specific medium and land use combinations which are used by risk managers as long-term targets during the analysis and selection of remedial alternatives. In addition, PRGs are often used early in site evaluations to determine if the concentrations of potential contaminants are present at concentrations that may pose an unacceptable risk to human health, in remedial investigation work plan development to develop the analyte list for samples that will be collected from a site, and in human health risk assessments to develop a final list of chemicals of potential concern.

The PRGs presented in this database were developed following the guidance in RAGS, Part B. RAGS, Part B, was prepared for risk assessors, remedial project managers, and others to assist them in developing PRGs for National Priorities List (NPL) sites. Specifically, RAGS, Part B, provides guidance on using United States Environmental Protection Agency (EPA) toxicity values and exposure information to derive risk-based PRGs that are protective of human health. Except where noted, the toxicity values used to derive the PRGs in the RAIS are based on the most current toxicological information from the Environmental Protection Agency's (EPA's) Integrated Risk Information System (IRIS)(EPA 1998) and the Health Effects Assessment Summary Tables (HEAST) (EPA 1997) and are updated on a monthly basis based on changes received from EPA. In the RAIS, the latest version of the PRGs is posted on the first screen viewed for user documentation. The risk-based PRGs in the database are applicable to all sites and, if used to guide early clean-up decisions, will result in residual risks from direct contact with a contaminated medium that satisfy the National Oil and Hazardous Substances Pollution Contingency Plan (NCP)(EPA 1990) requirements for protection of human health. Because the risk-based PRGs in the database were developed to protect human health, they may not be adequately protective of nonhuman receptors. For sites where risk-based PRGs for ecological receptors are required, a link to an ecological benchmarks risk analysis tools is provided and can be located at: <http://www.hsrdo.ornl.gov/ecorisk/ecorisk.html>.

In the RAIS, a user searches for a PRG(s) by selecting the chemical(s) and/or radionuclide(s) for which a PRG(s) is needed together with the applicable media, land use, and exposure route combination. To explore the derivation of the selected PRG(s), the user may link to a series of screens which display the equations and exposure parameters used to derive the selected PRG(s).

In the RAIS, PRGs are available for five landuse scenarios: agricultural, excavation, industrial, recreational, and residential. Refer to Figure 1. For each land use, decisions made to develop the landuse scenarios are presented. For each land use, the user may use default EPA exposure parameters to develop generic PRGs or modify the exposure parameters to develop site-specific PRGs. This feature allows the user to modify PRG calculations to meet region-specific guidance; ethnic, population, or stakeholder concerns; or any other considerations.

After deriving the generic or site-specific PRGs, the user may view the PRGs on the screen or download them in a tab or comma delimited file. The ability to download the PRGs in a format that can be easily imported into common spreadsheet or statistical computer programs is provided to expedite the risk assessment process and allow the user to easily accommodate their own computer software needs. Users can access the PRG tool at: http://risk.lsd.ornl.gov/prg/prg_document.html.

2.1 AGRICULTURAL LAND USE

For the agricultural land use, residents are assumed to raise and consume various farm products. Exposure routes include consumption of beef, consumption of whole milk, and consumption of vegetables. Equations used to calculate chemical-specific risk-based PRGs in farm products are presented as well as equations for soil and water that contribute contaminants to farm products. Equations for direct contact with contaminated soil and water or consumption of fish are not discussed in the agriculture land use but are addressed within the residential and recreational land uses, respectively. Because of the uncertainty inherent in defining the rates of consumption of all farm products simultaneously, PRGs combining consumption of all products are not presented.

In deriving chemical concentrations in farm products, various farming practices are defined in order to select various parameters. Because these practices tend to vary by region across the United States, the region used to define farming practices was the mid-south. Also, when deriving the chemical-specific risk-based PRGs for soil and water contributing contamination to farm products, it must be recognized that contamination can originate from either soil or water. If both the soil and water used in farm production are contaminated, then it is necessary to integrate the contributions from both when selecting the appropriate PRG. This presents a unique problem because chemical-specific risk-based PRGs are medium specific. To address this problem, the calculations presented in the RAIS provide the slopes and y-intercepts for an algebraic equation that describes the impact differing levels of water contamination have on the PRGs for soil, and the impact differing levels of soil contamination have on the PRGs for water. These calculations allow the user to solve for a PRG in one medium (e.g., water) while assuming a contaminant concentration in the other medium (e.g., soil).

The PRGs for soil and water are back-calculated using the PRGs for farm products. These equations include those for water contamination alone, soil contamination only, and soil and water contamination combined. These three sets of equations also evaluate vegetables, whole milk, and beef. The supporting equations which are used to calculate the concentration of a chemical concentration in a farm product given a concentration in soil and/or water are presented and include the chemical concentrations in vegetables, pasture (assuming no irrigation), beef, and milk. Special cases that should be considered when utilizing the PRG equations and the chemical-specific risk-based PRGs are also presented.

Finally, because the rate of milk consumption in the United States varies in relation to age and body weight, the calculations used to derive the PRGs based on carcinogenic risk due to milk consumption consider an age-adjusted consumption factor. For the same reason, the PRGs based on systemic toxicity (i.e., hazard) are calculated separately for the child and the adult.

Fig. 1. Land uses and exposure routes considered in the development of PRGs.

2.2 RESIDENTIAL LAND USE

For the residential land use, residents are assumed to be exposed to contaminated media on a daily basis over a lifetime. Exposure routes considered include the ingestion of ground or surface water, inhalation of ground or surface water during water use in the home, dermal contact with ground or surface water while showering, incidental ingestion of soil or sediment, inhalation of particulates and/or vapors emitted from soil or sediment, dermal contact with contaminated soil or sediment, and external exposure to ionizing radiation emitted from contaminants in soil or sediment. Equations used to solve for the chemical-specific risk-based PRGs for each of these exposure routes are presented for individual pathways and selected combinations.

The exposure assumptions utilized for this land use scenario result in the smallest, or most conservative, chemical-specific risk-based PRGs. As discussed earlier, the consumption of farm products and fish are presented in the agriculture and recreational land uses, respectively.

Because most radionuclides are not volatile, exposure to vapors emitted from ground or surface water are only considered for tritium and radon. Tritium is considered because it may exist as either hydrogen gas in water or replace one of the hydrogens found in the water molecule. Radon is considered because groundwater that is in contact with rock or soil containing radium will pick up radon-222 and release it to the atmosphere when the water is used.

For the soil and sediment exposure routes, the formula used in the RAIS assumes that there is an unlimited potential for surface erosion and the production of particulates and vapor emissions. Also because the rate of incidental ingestion of soil and sediment in relation to body weight varies significantly between children and adults, the calculation of the PRG based on carcinogenic risk due to incidental ingestion of soil is calculated using an age-adjusted ingestion factor. For the same reason, the PRGs based on systemic toxicity (i.e., hazard) are calculated separately for the child and the adult.

The equations used to develop some of the exposure parameters needed in the PRG equations are presented with the supporting equations and information as special cases. The user of the RAIS is encouraged to view these special cases before utilizing the PRG equations and the chemical-specific risk-based PRGs. A link is provided to each of these areas in multiple locations.

2.3 INDUSTRIAL LAND USE

For the industrial land use, adult workers are assumed to be routinely exposed to contaminated media within a commercial area or industrial site. Exposure routes considered include incidental ingestion of ground or surface water, incidental ingestion of soil or sediment, inhalation of particulates and/or vapors emitted by soil or sediment, dermal contact with contaminated soil or sediment, and external exposure to ionizing radiation emitted from contaminants in soil or sediment. As with the derivation of the residential PRGs for direct contact with soil or sediment, the calculations in the RAIS used to derive the industrial land use PRGs for inhalation of particulates and vapors emitted from soil or sediment assume that there is an unlimited potential for surface erosion and production of particulates and vapor emissions. Equations used to solve for the chemical-specific risk-based PRGs for each of these routes of exposure are presented considering each exposure route alone and considering the exposure routes simultaneously.

The equations utilized to develop some exposure parameters needed in the PRG equations are presented with supporting equations and information as special cases. The user of the RAIS is encouraged to view these special cases before utilizing the PRG equations and the chemical-specific risk-based PRGs and is provided links to these areas in multiple locations.

2.4 EXCAVATION LAND USE

For the excavation land use, individuals are assumed to be exposed to contaminated soil or sediment infrequently and for only a short period of time. Exposure routes considered include the incidental ingestion of soil or sediment, inhalation of particulates and/or vapors emitted by soil or sediment, dermal contact with contaminated soil or sediment, and external exposure to ionizing radiation emitted from contaminants in soil or sediment.

When using these equations, the user should be aware of certain considerations which are presented in the special cases section. In particular, due to weather considerations for this scenario, exposure frequency is assumed to be one month of the worker year, and, because excavation is assumed to be a rare occurrence, the exposure duration for any one worker is assumed to be for one year. Additionally, the calculations in the RAIS assume that there is an unlimited potential for soil erosion and production of particulate and vapor emissions. Finally, because the exposure durations are limited, the PRGs are calculated using subchronic reference doses (RfDs) for all exposure routes.

Equations used to solve for the chemical-specific risk based PRGs in soil or sediment are presented. Equations are shown for each of the exposure routes alone and for simultaneous consideration of all exposure routes. The equations utilized to develop some of the exposure parameters needed in the PRG equations are also presented with supporting equations and information.

2.5 RECREATIONAL LAND USE

The final land use evaluated is the recreational land use. Under this land use, individuals are assumed to be exposed to contaminated media while playing, hiking, or engaging in other outdoor activities. This use also includes what is often described as a "trespasser" or "site visitor" scenario in some risk assessments. Exposure routes considered include incidental ingestion of surface water, dermal contact with surface water, incidental ingestion of soil or sediment, inhalation of particulates and/or vapors emitted from soil or sediment, dermal contact with contaminated soil or sediment, external exposure to ionizing radiation emitted from contaminants in soil or sediment, and consumption of fish.

Particular considerations for recreational land use are also presented. For the soil and sediment pathways, it is assumed that there is an unlimited potential for surface erosion and the production of particulates and vapor emissions. In addition, because the rate of incidental ingestion of soil and sediment ingestion in relation to body weight varies significantly between children and adults, the calculation of the PRG based on carcinogenic risk due to direct ingestion of soil is calculated using an age-adjusted ingestion factor. For the same reason, the PRGs based on systemic toxicity (i.e., hazard) are calculated separately for the child and the adult. Furthermore, the equations solving for PRGs for fish are presented for both the chemical concentration in fish and the chemical concentration in surface water. Additional information concerning these calculations is also presented within the special cases area.

Equations are shown for when each of the exposure routes is considered alone and when all exposure routes are considered simultaneously. Special cases beyond those highlighted above that should be considered when utilizing the PRG equations and the chemical-specific risk-based PRGs are also presented.

3. REGULATORY LIMITS

Under the Comprehensive Environmental Response, Compensation, and Liability Act of 1980, as amended (CERCLA), the CERCLA Compliance Policy was enacted. (EPA 1989) This policy specified that Superfund remedial actions meet any federal standards, requirements, criteria, or limitations determined to be legally applicable or relevant and appropriate requirements (i.e., ARARs). Also included was a provision that promulgated state ARARs must be met if they are more stringent than federal requirements. This provision required both federal and state ARARs to be considered for Superfund sites. This system includes those established regulatory limits for surface water and groundwater.

The regulatory limits for surface water and groundwater contained in the RAIS database comprise chemical-specific PRGs based on potential Applicable or Relevant and Appropriate Requirements (ARARs). These values should be used in conjunction with risk-based PRGs to ensure that the PRGs for a site meet the residual risk requirements for protection of human health and the environment in the NCP. In some cases, the values presented in the RAIS may be To-Be-Considered (TBC) Guidance because these values are superseded by site-specific state requirements. The database currently contains federal limits and state limits from Kentucky, Ohio, and Tennessee. Additional states and other limits will be added as the RAIS is further developed and on special request.

The RAIS regulatory limits database has undergone extensive quality assurance reviews and has been updated on an annual basis based on new federal and state regulations. The user can retrieve the guidelines simply by selecting the boxes next to the appropriate parameters and marking the desired analyte name and/or Chemical Abstracts Service (CAS) registry number. The results for the search are available on screen in table format with associated references highlighted. Examples of some of the selections currently available in the system include:

- 1) Federal and State Primary Drinking Water MCLs
- 2) Federal Primary Drinking Water MCLGs
- 3) Proposed Federal Primary Drinking Water MCLs
- 4) Proposed Federal Primary Drinking Water MCLGs
- 5) Federal and State Primary Drinking Water MCLs (Radionuclides)
- 6) Federal and State Primary Drinking Water Proposed MCLs (Radionuclides)
- 7) Federal Secondary Drinking Water SMCLs
- 8) State Secondary Drinking Water SMCLs
- 9) State Human Water Supply Source
- 10) State Human Health WQC for Protection of Human Health from the Consumption of Fish Tissue Only
- 11) State Warm Water Aquatic Habitat WQC - Acute
- 12) State Warm Water Aquatic Habitat WQC - Chronic
- 13) State Radionuclide-Specific Minimum Surface WQC
- 14) Federal Human Health WQC for Aquatic Organisms and Drinking Water
- 15) Federal Human Health WQC for Aquatic Organisms Only
- 16) Federal Freshwater WQC - Maximum
- 17) Federal Freshwater WQC - Continuous

As noted earlier, in the future this portion of the RAIS will be expanded to include additional state regulations. The ultimate goal of this portion of the RAIS is to develop a national registry for all state guidelines. The regulatory limits database can be accessed at:
http://risk.lsd.ornl.gov/guide/reg_limits.html.

4. TOXICITY AND CHEMICAL FACTORS

The Toxicity and Chemical Factors include toxicity profiles, toxicity values and chemical-specific factors. Each of these are discussed in the following subsections.

4.1 TOXICITY PROFILES

The toxicity profiles in this database were developed using information taken from the EPA's IRIS and HEAST and other literature sources. The profiles and their references are provided to eliminate the effort needed to produce the toxicity profiles presented in the toxicity assessment chapter of a risk assessment and to supplement the human health risk-based PRGs presented elsewhere in the RAIS.

The toxicity profiles summarize the toxic effect associated with exposure to a chemical and the concentrations at which the adverse effects are expected to occur in humans. A general outline used in these profiles is as follows:

EXECUTIVE SUMMARY

- 1. INTRODUCTION**
- 2. METABOLISM AND DISPOSITION**
 - 2.1 ABSORPTION**
 - 2.2 DISTRIBUTION**
 - 2.3 METABOLISM**
 - 2.4 EXCRETION**
- 3. NONCARCINOGENIC HEALTH EFFECTS**
 - 3.1 ORAL EXPOSURES**
 - 3.2 INHALATION EXPOSURES**
 - 3.3 OTHER ROUTES OF EXPOSURE**
 - 3.4 TARGET ORGANS/CRITICAL EFFECTS**
- 4. CARCINOGENICITY**
 - 4.1 ORAL EXPOSURES**
 - 4.2 INHALATION EXPOSURES**
 - 4.3 OTHER ROUTES OF EXPOSURE**
 - 4.4 EPA WEIGHT-OF-EVIDENCE**
 - 4.5 CARCINOGENICITY SLOPE FACTORS**
- 5. REFERENCES**

In the database, the toxicity profiles are presented in two formats: formal and condensed. Toxicity profiles in the formal format are several pages long and are similar to the profiles found in IRIS. For this reason, a WordPerfect file of the formal toxicity profile is available for downloading (see the beginning of the formal toxicity profile). Toxicity profiles in the condensed format are generally less than a page in length and are suitable for use as a toxicity profile in the toxicity assessment chapter of a human health risk assessment. Users of the RAIS may choose to initially view the condensed versions and then link back to either other profiles or directly to the formal version of the viewed profile. A cautionary statement and associated link is included in this area to notify the user to consult the Toxicity Value Database, which is updated monthly, to ensure that current toxicity values are included within the profiles. The toxicity profiles can be accessed using the following address:
http://risk.lsd.ornl.gov/tox/rap_toxp.htm.

4.2 TOXICITY VALUES

The Toxicity Values database contains the human health toxicological information needed to perform risk evaluations and assessments. The toxicity values contained in this database were developed specifically for use in risk evaluations and assessments utilizing methods presented in RAGS. The database has also been compiled using information from the EPA's IRIS and HEAST and from other necessary information sources. The values are updated on a monthly basis based on changes received from EPA, and the date of the latest version is posted on the first screens viewed. Information contained in the database is referenced and supplemental information is provided. This information is available at: http://risk.lsd.ornl.gov/tox/tox_values.html.

The user is given the option to search the database for chemical-specific information and to either view this information on screen in table format or to download the information as an Excel spreadsheet. This capability reduces the time spent by users converting the information to other formats and helps prevent user error. In addition, the user may refer to the specific area entitled "Using Toxicity Values in Risk Assessments". This link provides information regarding the special cases within the toxicity values database and describes how the toxicity values should be utilized.

The toxicity database contains a variety of information that is used to either calculate risks or hazards (e.g., cancer slope factors and reference doses, respectively) or to derive dose estimates (e.g., volatilization factor). The database contains two levels of organization; these are nonradionuclides and radionuclides. Nonradionuclides are defined as chemicals that do not undergo nuclear decay and emit ionizing radiation. For example, the inorganic chemicals calcium, carbon, manganese, and iron are nonradionuclides. In addition, the organic compounds trichloroethene, carbon tetrachloride, etc. are also nonradionuclides. The radionuclides are defined as chemicals that do undergo nuclear decay and emit ionizing radiation. For example, the isotopes of uranium, uranium-235 (^{235}U), uranium-236 (^{236}U), and uranium-238 (^{238}U) are radionuclides.

4.2.1 NONRADIONUCLIDE CHEMICAL INFORMATION

Within the nonradionuclide level of organization, chemicals are divided into two broad categories. These categories are inorganic and organic compounds. The inorganic chemicals are defined as chemicals or compounds that do not contain a carbon skeleton. For example, manganese, mercury, and iron are inorganic chemicals. Organic compounds are defined as chemicals or compounds that do contain a carbon skeleton. For example, trichloroethene, benzo(a)pyrene, and acetone are organic compounds.

Although the database can be searched by levels of organization and categories, a more useful search in most applications is by either chemical name or CAS number. When searching by chemical name, care must be taken because organic compounds, and some inorganic chemicals, are often called by more than one name. For example, 2-butanone is also called methyl ethyl ketone, methyl acetone, 2-oxybutane, or simply MEK, depending on the chemical application. To assist the user of this database to determine the appropriate chemical name, a link to "ChemFinder" is provided. This service allows the user to determine synonyms for chemicals and compounds and learn about their chemical characteristics.

As noted earlier, for each chemical or compound a variety of information is provided. However, in some cases, information may be lacking for a chemical or compound. Reasons for this include that the information is not applicable to that chemical or compound or that the information is not available at this time. Toxicity information that is currently available in the database includes:

- 1) Chemical name—the common name of the chemical or compound. Usually as defined in either IRIS or HEAST.
- 2) CAS number—the Chemical Abstracts Service Registry Number.
- 3) Reference Dose (RfD)—for those chemicals eliciting a toxic response, the oral chronic RfD, dermal chronic RfD, oral subchronic RfD, dermal subchronic RfD, inhalation chronic RfD, inhalation chronic RfD, and inhalation subchronic RfD are provided.

- 4) Cancer slope factor—for those chemicals which are carcinogens, the oral slope factor, inhalation slope factor, and dermal slope factor are provided.
- 5) EPA Classification—the cancer classification of the chemical or compound assigned by EPA.
- 6) Date withdrawn—the date which a toxicity value was withdrawn by EPA, if applicable. For withdrawn values, the most recent value prior to withdrawal is included in the database if prior approval has been received by Region 4.

Other chemical-specific information that is available in the database includes:

- 1) Volatilization factor (VF)—an estimate of the rate at which a chemical is emitted from soil as a vapor.
- 2) Soil saturation concentration (C_{sat})—an estimate of the maximum concentration of a chemical that may exist in soil before free product is present.
- 3) Gastrointestinal absorption factor (GIAF)—an estimate of the rate at which a chemical or compound is absorbed from the gastrointestinal tract of a human.
- 4) Dermal absorption factor (ABS)—an estimate of the rate at which a chemical is partitioned between the skin and a solid medium such as soil.
- 5) Permeability constant (K_p)—an estimate of the rate at which a chemical is partitioned between the skin and water.
- 6) Beef transfer coefficient (F_b)—an estimate of the rate at which a chemical is transferred from soil or water through beef to humans as beef is consumed.
- 7) Fish bioaccumulation factor (BF)—an estimate of the rate at which a chemical is accumulated from water into the tissue of fish.
- 8) Milk transfer coefficient (F_m)—an estimate of the rate at which a chemical is transferred from soil or water through a cow to humans as milk is consumed.
- 9) Soil-to-Plant dry uptake factor (Bv_{dry})—an estimate of the rate at which a chemical in soil or water moves into plant tissues on a dry weight basis.
- 10) Soil-to-Plant wet uptake factor (Bv_{wet})—an estimate of the rate at which a chemical in soil or water moves into plant tissues on a wet weight basis.
- 11) Henry's Law Constant (H)—an estimate of the extent of chemical partitioning between air and water and equilibrium. A larger value indicates that the chemical is more likely to volatilize.
- 12) Molecular weight (MW)—the weight of the chemical.
- 13) Organic carbon partition coefficient (K_{oc})—an estimate of the extent of chemical partitioning between organic carbon and water at equilibrium. A larger value indicates that the chemical is more likely to remain bound to soil or sediment.
- 14) Octanol-water partition coefficient (K_{ow})—an estimate of the extent of chemical partitioning between water and octanol at equilibrium. A larger value indicates that the chemical is more likely to partition to octanol and, by analogy, more likely to be bioconcentrated in aquatic organisms.

Footnotes for withdrawn, provisional, or derived toxicity values are included in the system. The user may consult with the area entitled "Using Toxicity Values in Risk Assessments" for specific information concerning these values.

4.2.2 RADIONUCLIDE INFORMATION

Much of the chemical characteristics information contained in the database for radionuclides is similar to that for chemicals. In the radionuclide portion of the database, toxicity values for ingestion, inhalation, and external exposure are presented. In all cases, the only values presented are those for carcinogenesis (i.e., slope factors). If a RfD for a radionuclide is needed, the user should access the RfD for the inorganic chemical in the nonradionuclide portion of the database. For example, the radionuclide portion of the database contains ingestion, inhalation, and external exposure slope factors for each

uranium isotope (e.g., ^{234}U , ^{235}U , ^{236}U , ^{237}U , ^{238}U); however, the radionuclide portion of the database does not contain RfDs for these isotopes even though exposure to uranium may cause elicit a systemic toxic response. If the user requires an RfD for any of the uranium isotopes, the RfD for "Uranium (Soluble Salts)" should be used. This value is contained in the nonradionuclide portion of the database.

All slope factors contained in the radionuclide database were calculated by the EPA's Office of Radiation and Indoor Air (ORIA). These values were derived by ORIA using methods for estimating radiogenic cancer risks. A detailed discussion of ORIA's approach and assumptions for this methodology is presented in *Estimating Radiogenic Cancer Risks* (EPA 1993).

For some radionuclides, two sets of slope factors are presented. For example, in the database there is a set of slope factors for ^{235}U and a set of slope factors for $^{235}\text{U} + \text{D}$. In these cases, the set of slope factors for the radionuclide is used when estimating risk from exposure to pure radioisotope, and the set of slope factors for radionuclide + D is used when estimating risk from exposure to the radioisotope and its short-lived radioactive decay daughter products (i.e., those decay products with radioactive half-lives less than or equal to 6 months—see HEAST).

It should be noted that a slope factor for dermal contact is not included in the radionuclide portion of the database. These have not been included because they are not available, and because EPA has concluded that dermal exposure is generally not an important route of exposure for radionuclides (RAGS, 1989). The only additional chemical-specific parameter contained in the radionuclide portion of the database that is not contained in the nonradionuclide portion of the database is radioactive half-life (T_R). This value is provided to assist the risk assessor determine the importance of radioactive decay and daughter ingrowth in the risk evaluation.

4.3 CHEMICAL-SPECIFIC FACTORS

The database of chemical-specific factors contains a subset of the information included in the Toxicity Values database along with the radioactive half-lives. Therefore, these values are also needed in the human health risk assessment exposure equations to calculate dose or in the human health risk-based PRGs equations to calculate the chemical-specific risk-based PRGs. This database contains information taken from a variety of sources, and these sources are referenced.

The chemical-specific factors contained in this database were also developed for use in risk evaluations and assessments performed utilizing methods presented in RAGS. Individuals intending to use these values with methods not consistent with RAGS should consult with risk assessment professionals, including those at their regulatory agencies.

Once again to use this database, the user will choose:

- (1) the chemical-specific parameters (chemical-specific factors),
- (2) the analytes by either name or CAS number, and
- (3) an output option.

For output options, the user may view the results on screen, view the results on screen with references, or download the information in a tab or comma delimited file. Users may access this information by choosing 'Chemical Specific Factors' at http://risk.lsd.ornl.gov/homepage/rap_tool.htm.

5. HUMAN HEALTH RISK EXPOSURE MODELS

The human health risk exposure model tool calculates doses and risks from exposure concentrations. Users of this tool can calculate the doses and risks by either supplying a data set of concentrations (Limited Access) or selecting chemicals and hand-entering exposure concentrations. Currently only SAS datasets and SAS transport files can be directly uploaded and used by the risk equation tool; however, other file formats need only be modified to be utilized by the system. Requirements and a point of contact for uploading a SAS data set or for questions are supplied. To use this tool, the land use and exposure combinations for a site must be selected, and a sort order for the final output must be chosen. After selecting the land use and exposure combinations, the user may modify exposure parameters within the dose equations to develop site-specific doses and risks or may utilize the default exposure parameters provided. The results of these choices can be output to the screen or to a comma delimited file.

The dose equations utilized by this tool are based on guidance in RAGS and RAGS, Part B. In addition, this tool contains some equations developed for assessment of sites on the Oak Ridge Reservation in Oak Ridge, Tennessee and approved by EPA, Region 4. Under "special cases" a complete description of what may be specific to the Oak Ridge Reservation is included. Additional discussion of these special cases and the strategy used for risk assessment at the Oak Ridge Reservation is presented in *Risk Assessment Strategy at DOE-ORO* (LMES, 1996). It is suggested that all RAIS users read the special cases before using this tool. General references for the entire tool can be accessed simply by linking to references or the more specific parameter references are located in the equation tables.

The user may select risk equations by the following land use and media options:

1. Excavation Land Use; Exposure to Contaminants in Soil
2. Industrial Land Use; Exposure to Contaminants in Soil
3. Recreational Land Use; Exposure to Contaminants in Soil
4. Recreational Land Use; Exposure to Contaminants in Water
5. Residential Land Use; Exposure to Contaminants in Soil
6. Residential Land Use; Exposure to Contaminants in Water

Land use and media combinations available in the human health risk exposure models are the same as those available for the PRG tool. Refer to Figure 1 for a detailed view of the available equations. Users can access this tool at http://risk.lsd.ornl.gov/prg/for_sel_data.html.

6. ECOLOGICAL BENCHMARKS

The ecological benchmarks tool contains not only benchmarks but other tools and applications widely used to conduct ecological screening and baseline risk assessments. For this particular tool, users can register for future update notices about this site. This site is located at: <http://www.hsrdo.ornl.gov/ecorisk/ecorisk.html>.

Risk assessments of waste sites require that contaminants be screened to identify those chemicals that may pose an ecological hazard. A screening assessment involves a comparison of the reported environmental levels of the contaminants with toxicological benchmarks derived from laboratory or field data for a particular species or group of organisms. If a chemical concentration or the estimated exposure level is lower than the lowest calculated benchmark, then the chemical is unlikely to represent an ecological risk. However, if the chemical concentration or the reported detection limit exceeds a

benchmark, then further analysis is needed to determine what, if any, hazard is posed by that chemical. The more the chemical concentration exceeds the benchmark value, the more likely that the contaminant poses an ecological risk. Screening benchmarks, therefore, provide a quick way to prioritize contaminants at a particular waste site.

This tool contains information that can be used to conduct ecological screening and baseline risk assessments at hazardous waste sites. Chemical-specific information on screening benchmarks is presented in five background reports: (1) aquatic biota; (2) terrestrial wildlife (mammals and birds); (3) terrestrial plants; (4) sediment-associated organisms; and (5) soil invertebrates and microbial processes. These reports vary in size and scope because of the limitations in the basic toxicological data from which benchmarks were derived. The chemicals evaluated in these reports were originally selected from a list of contaminants identified at DOE's Oak Ridge facility. As more information becomes available, the reports have been expanded to include other contaminants. In addition, benchmarks will change and new benchmarks will be added as more information becomes available.

This site also contains documents outlining methods, tools, and guidance for conducting various aspects of ecological risk assessment. In addition, complete text copies of ecological risk assessment reports for specific DOE sites are available. Screening Benchmarks Reports can be downloaded in portable document format (PDF) or WordPerfect format. Appropriate directions for downloading and viewing these files are provided.

7. RISK RESULTS

Site-specific information for the Department of Energy Oak Ridge Operation is also being made available through the homepage of the ORO Risk Assessment Program at http://risk.lsd.ornl.gov/rap_hp.htm. This area provides prioritization information, risk assessments results, and site photographs and maps.

Currently, the prioritization area contains Release Site Maps which are based on the Environmental Management (EM)-40 Release Site Methodology. These maps indicate low, medium, high, and no further action for the available sites. Most of the maps have been divided into sections denoted by black lines. The user is able to select a section to see an enlarged map and to gain information concerning the release sites. Future plans include adding the ORO site prioritization methodology and database.

In the risk assessment area, a list of site screening and baseline risk assessment reports is provided along with appropriate contacts for obtaining this information. In addition, the risk results from these reports are provided graphically where available and in different formats, indicating high risk areas using various risk criteria.

The final area links are to site descriptions and maps. This area is beneficial for understanding the complete make-up of a site. The user can become familiar with a site by viewing the site photographs or by reading the extensive site descriptions.

Each of these areas provide a great resource for additional sites to be added. This type of information is easily viewed and used by the public user and can provide project managers with easily accessed information about specific risk assessment results. This option allows the user to graphically view risk results obtained in the remedial investigation process without having to research volumes of documents to understand the risk picture.

8. OTHER INFORMATION

Work is currently underway to update the RAIS to include additional tools and features. A placemaker has already been added to most of the tools to include a tutorial. The tutorials would guide users who are not experienced in the field of risk assessment through the derivation and use of specific tools. These tutorials would also be used to answer the most commonly asked questions about each of the RAIS tools. An example of these tutorials is that developed by ORNL and entitled "What is Risk Assessment." This tutorial is available from the CRE web site at http://www.doe.gov/riskcenter/cre_what.html or from ORNL's Risk Assessment Program homepage at http://risk.lsd.ornl.gov/rap_hp.htm.

Additional communication and training tools will also provide users with information necessary to understand the entire risk assessment process which is not covered in specific application tools. For example, tutorials on communicating risk information to the stakeholders involved in the remediation process and on incorporating risk assessment into the data quality objective process may be added.

9. REFERENCES

EPA (United States Environmental Protection Agency). 1989. *Risk Assessment Guidance for Superfund: Volume 1-Human Health Evaluation Manual (Part A)*, EPA/540/1-89/002, Office of Emergency and Remedial Response, Washington, D.C.

EPA. 1990. *National Oil and Hazardous Substance Pollution Contingency Plan*, Federal Register 55, No. 46.

EPA. 1991. *Risk Assessment Guidance for Superfund. Volume 1-Human Health Evaluation Manual (Part B, Development of Risk-based Preliminary Remediation Goals)*, OSWER Directive 9285.7-01B, Office of Emergency and Remedial Response, Washington, D.C.

EPA. 1993. *Estimating Radiogenic Cancer Risks*, 402-R-93-076, Office of Radiation and Indoor Air (ORIA), Washington, D.C.

EPA. 1997. *Health Effects Assessment Summary Tables, FY 1997 Update*, EPA 540/R-97-036, Office of Research and Development and Office of Emergency and Remedial Response, Washington, D.C.

EPA. 1998. *Integrated Risk Information System (IRIS)*, Office of Research and Development, National Center for Environmental Assessment, Cincinnati, OH.

LMES (Lockheed Martin Energy Systems, Inc.). 1996. *Risk Assessment Strategy at DOE-ORO*, ES/ER/TM-180, Oak Ridge National Laboratory, Oak Ridge, TN.

INTERNAL DISTRIBUTION

1. L. D. Bloom	8. B. E. Sample
2. R. R. Bonczek	9. Central Research Library
3. F. G. Dolislager	10. ORNL Laboratory Records-RC
4. S. B. Kerr	11-12. ORNL Laboratory Records-OSTI
5. M. L. Land	
6. P. Y. Lu	
7. C. W. McGinn	

EXTERNAL DISTRIBUTION

13. M. E. Bollinger, Department of Energy, 9800 S. Cass Avenue, Bldg. 201, Argonne, IL 60439
14. A. J. Kuhaida, Bechtel Jacobs Inc. LLC, ETPP, Bldg. K-1007, Oak Ridge, TN 37830
15. T. L. Mims, Department of Energy, P.O. Box 2001, Oak Ridge, TN 37831
16. R. M. Pawlowicz, Bechtel Jacobs Inc. LLC, 151 Lafayette, Oak Ridge, TN 37830
17. T. C. Perry, Department of Energy, P.O. Box 2001, Oak Ridge, TN 37831
18. M. Acke Ramicone, Department of Energy, 9800 S. Cass Avenue, Bldg. 201, Argonne, IL 60439
19. P. R. Siebach, Department of Energy, 9800 S. Cass Avenue, Bldg. 201, Argonne, IL 60439
20. A. L. Young, Department of Energy, 9800 S. Cass Avenue, Bldg. 201, Argonne, IL 60439