RESRAD-ECORISK: A COMPUTER CODE FOR ECOLOGICAL RISK ASSESSMENT

ABSTRACT
RESRAD-ECORISK is a PC-based computer code developed by Argonne National Laboratory (ANL) to estimate risks from exposure of ecological receptors at sites contaminated with potentially hazardous chemicals. The code is based on and is consistent with the methodologies of RESRAD-CHEM, an ANL-developed computer code for assessments of human health risk. RESRAD-ECORISK uses environmental fate and transport models to estimate contaminant concentrations in environmental media from an initial contaminated soil source and food-web uptake models to estimate contaminant doses to ecological receptors. The dose estimates are then used to estimate a risk for the ecological receptor and to calculate preliminary soil guidelines for reducing risks to acceptable levels. Specifically, RESRAD-ECORISK calculates (1) a species-specific applied daily dose for each contaminant (using species-specific life history information and site-specific environmental media concentrations), (2) an ecological hazard quotient (EHQ) for each contaminant and species, and (3) preliminary soil cleanup criteria for each contaminant and receptor. RESRAD-ECORISK incorporates a user-friendly menu-driven interface, databases and default values for a variety of ecological and chemical parameters, and on-line help for easy operation. The code is sufficiently flexible to simulate different contaminated sites and incorporate site-specific ecological data.

INTRODUCTION
Assessment of ecological risks at contaminated sites is more complicated than assessment of human health risks for a number of reasons. Ecological systems are extremely complex, containing multiple species with differing physiologies, behaviors, and life histories; and the range of effects (endpoints) may vary greatly depending on the species and contaminants present at a site. For example, in addition to mortality the effects of contaminant exposure may include habitat loss, reduced population size, altered community structure, and changes in ecosystem structure and function. In addition, quantitative ecological risk assessments typically employ tissue analysis and toxicity testing to evaluate contaminant exposure and effects. However, these approaches often require destructive sampling of biota (Cobb and Hooper 1994), and such sampling is not possible for many of...
the species that occur at contaminated sites. Some species, such as the bald eagle, are protected by federal and state laws and cannot be sacrificed for laboratory analysis. Thus, the need clearly exists for a comprehensive computer model for ecological risk assessment. Although several computer codes have been developed for human health risk assessment, computer models for ecological risk assessments are much less common (e.g., Vandergrift and Ambrose 1988; Connolly and Thomann 1985).

RESRAD-ECORISK is a PC-based computer code developed to estimate risks from contaminant exposure to ecological receptors without the need for destructive biological sampling and using site-specific contaminant data that is typically collected during site characterization activities. The code is derived from RESRAD-CHEM, a human health risk assessment computer model developed by ANL (Cheng 1993). RESRAD-ECORISK uses species-specific exposure parameters and site contaminant data, together with food web and fate and transport models, to calculate an applied daily dose (ADD) and an ecological hazard quotient (EHQ) for ecological receptors using a chemically contaminated site. The code then uses the ADD and EHQ estimates to derive soil cleanup criteria for individual chemicals, receptors, within the user-specified time frame.

A schematic representation of RESRAD-ECORISK showing contaminant pathways to ecological receptors is shown in Figure 1. RESRAD-ECORISK estimates contaminant concentrations within species-specific compartments of the pathways by using contaminant transfer factors, bioaccumulation factors, a soil-groundwater leaching model, and a soil-air volatilization model. Because RESRAD-ECORISK and RESRAD-CHEM use the same environmental fate and transport models, the predicted environmental media concentrations for a given site are consistent between both models and risk assessments. From the risk assessment perspective, this consistency in methodology is a desirable feature when conducting a baseline risk assessment that includes both human health and ecological concerns.

The RESRAD-ECORISK code uses a menu-driven interface from which the user can easily access the data input screens, modify databases, run the RESRAD-ECORISK calculations, and view the output. The input parameters have default values that are either empirically based or represent carefully selected reasonable conservative values. However, site-specific parameter values, if available, may be input directly. Databases of contaminant-specific parameters are provided for 151 chemicals on the U.S. Environmental Protection Agency’s Target Compound List for Organics (TCL) (EPA 1991a) and Target Analyte List for Inorganics (TAL) (EPA 1991b). The parameters in these databases include soil-to-plant uptake factors, insect bioaccumulation factors, chemical parameters such as Henry’s law constants and molecular diffusion coefficients, and benchmark values for the ecological receptors. RESRAD-ECORISK allows users to access and modify these databases as needed to include site-specific chemical data.
Figure 1. Schematic representation of contaminant transport, fate, and uptake as evaluated by RESRAD-ECORISK

ECOLOGICAL RECEPOTRS MODELED IN RESRAD-ECORISK

Currently, RESRAD-ECORISK will calculate an ADD, an EHQ, and soil guidelines for five terrestrial vertebrate receptors: the American robin, the mallard duck, the whitetailed deer, the eastern cottontail, and the deer mouse. These are five common species throughout large portions of the United States, and can be reasonably expected to exist at many Department Of Energy (DOE) sites. Contaminant uptake models incorporating multiple exposure and uptake are included in RESRAD-ECORISK for these species, and these models are used to estimate dose and risk. For each of these receptors, the code includes information on body weight; ingestion rates for food, water, and soil; home range; and diet composition. The user is able to select any combination of receptors for analysis in a single operation. Uptake models for additional species are under development and will be added to the code as they are completed. These additional receptors will include amphibians and reptiles, as well as birds and mammals that occupy the top of food chains.
CONTAMINANT UPTAKE PATHWAYS CONSIDERED IN RESRAD-ECORISK

RESRAD-ECORISK incorporates six contaminant uptake pathways for the ecological receptors (Figure 1). These pathways are (1) ingestion of terrestrial vegetation, (2) ingestion of aquatic vegetation, (3) ingestion of insects, (4) ingestion of incidental sediment, (5) ingestion of incidental soil, and (6) ingestion of water. Pathways for the American robin are the ingestion of terrestrial vegetation, soil, insects, and water. The pathways for the mallard duck include ingestion of aquatic vegetation, sediment, insects, and water. For the white-tailed deer, contaminant uptake is considered to occur along two pathways, ingestion of terrestrial vegetation and water. Pathways for the eastern cottontail include ingestion of terrestrial vegetation, soil, and water, and, finally, ingestion of terrestrial vegetation and ingestion of soil are considered for the deer mouse.

To estimate the ADD from any dietary pathway, RESRAD-ECORISK uses the following equation (EPA 1993):

\[ \text{ADD}_k = (C_k \cdot DF_k \cdot SU \cdot NIR_k) \]

where:
- \( \text{ADD}_k \) = applied daily dose (mg/kg-day),
- \( k \) = pathway index,
- \( C_k \) = average contaminant concentration (mg/kg),
- \( DF_k \) = fraction of the total diet (unitless),
- \( SU \) = site-use factor
- \( NIR_k \) = normalized ingestion rate,
- \( \text{SU} \) = site-use factor
- \( \text{IR} \) = normalized ingestion rate (IR) (gm/day)] \div [body weight (BW) (gm)].

A similar equation is used to estimate the ADD from the drinking water pathway. The ADD from all the pathways are summed to provide a total estimated ADD.

Individual contaminant uptake pathways can be selected or suppressed by the user according to the individual receptors and to the site-specific ecological conditions. For example, the diet of the American robin is almost exclusively insects in spring while in summer it consists of about equal portions of insects and plant matter such as fruits and berries (EPA 1993). RESRAD-ECORISK permits the user to inactivate the terrestrial vegetation pathway for the American robin to more accurately estimate a spring ADD. If a pathway is suppressed, RESRAD-ECORISK automatically suppresses the nonapplicable input parameters. This procedure simplifies the data input effort and reduces the calculation time.
Figure 2. Example computer screen within RESRAD-ECORISK showing exposure parameters for the American robin

**SPECIES-SPECIFIC EXPOSURE FACTORS**

The species-specific information used in the uptake models to estimate the ADD includes total ingestion rate, diet (fraction of total diet consisting of vegetation, insects, and soil), body weight, and home range. Ingestion rates of vegetation, insects, and soil are estimated by multiplying the diet fractions by the total ingestion rate. The code provides default values (from the EPA *Wildlife Exposure Factors Handbook* [EPA 1993]) for the diet fractions, but site-specific information may be entered instead if available. Figure 2 shows an input screen of exposure factors for the American robin. The food and water ingestion rates can be input directly from the code or calculated by the code using allometric equations (Nagy 1987), which estimate an ingestion rate from the average body weight of the species.
Figure 3. Example computer screen within RESRAD-ECORISK showing benchmark values for the American robin for three metals and one volatile organic compound.

The site-use factor is a site- and species-specific parameter that takes into account the size of the contaminated zone and the home range of the species. The site-use factor represents the proportion of time the species spend in the contaminated area and is used to estimate the proportion of daily intake originating from the contaminated area.

**BENCHMARK VALUES**

Benchmark values contained in the RESRAD-ECORISK database represent no-observed-adverse-effects levels (NOAEL) by considering total uptake of water and food for each chemical and receptor. The benchmark values were obtained from a variety of sources in the open scientific literature as well as from DOE, EPA, and other agency reports (e.g., Opresko et al., 1994). Figure 3 shows an input screen of American robin benchmark values.
Benchmark values are not provided for all of the chemicals included in the database; however, the user may input a benchmark value for any chemical included. The separate benchmark values for diet and water listed to the right of the total benchmark are not used in the RESRAD-ECORISK calculations. However, they may be substituted by the user in place of the total benchmark value if the user is analyzing risk from only the diet uptake pathway(s) or only the water uptake pathway for a receptor.

ESTIMATION OF THE ECOLOGICAL HAZARD QUOTIENT

Estimation of the EHQ requires the use of benchmark values that represent contaminant concentrations considered to represent little or no risk to a receptor. The EHQ is analogous to the "environmental effects quotient" identified by EPA Region 3 for ecological risk estimation (Davis 1994), and the quotient (or ratio) method used by the EPA Office of Pesticide Programs to estimate risks from pesticides (Barton 1994). The EHQ is predicted for each contaminant and receptor by taking the ratio of the ADD to the NOAEL benchmark value:

\[ \text{EHQ} = \frac{\text{ADD}}{\text{Benchmark NOAEL}} \]

where:
- \( \text{EHQ} \) = ecological hazard quotient (unitless),
- \( \text{ADD} \) = estimated applied daily dose (mg/kg/day),
- \( \text{Benchmark NOAEL} \) = an applied daily dose reported to produce no adverse effect in the receptor species (mg/kg/day).

Values of the EHQ may vary from 0 to infinity, and values greater than 1.0 are considered to demonstrate a potential risk to the receptor from the predicted ADD. Values between 1.0 and 10.0 indicate a slight potential risk of adverse effects from the estimated ADD, values between 10.0 and 100.0 indicate moderately high potential risk, and values greater than 100 indicate extreme risk from the predicted ADD.

INPUT DATA FOR SITE CHARACTERIZATION

The input data required by RESRAD-ECORISK for the fate and transport models include the physical, hydrological, geochemical, and meteorologic data for the contaminated site. The code uses these parameters, to adjust the source of the contamination over time to account for leaching, volatilization, erosion, and mixing. RESRAD-ECORISK uses a box model to predict on-site air concentrations and a one-dimensional model to calculate on-site water concentrations.

Physical data required by the code include the size and depth of the contaminated soil.
zone and the densities and porosities of different soil layers beneath this zone. Up to five uncontaminated, unsaturated soil layers under the contaminated zone are allowed in RESRAD-ECORISK, and these soil layers can be of different depths and properties.

Required hydrological data include soil conductivity, saturated zone hydraulic gradient, soil b parameters, and water table depth. The soil b parameters are used to calculate the saturation ratios of different soil layers, which are then used to calculate the retardation factors of chemicals.

Geochemical data required are mainly the soil and water distribution coefficients (Kd) of chemicals. In addition to direct input of Kd values, the user can select among four options to derive the Kd values. The first option allows the user to input groundwater concentrations that have been measured at the same time as the soil concentration and to input an elapsed time since the contamination occurred at the site. RESRAD-ECORISK uses these parameters to derive a Kd value for the chemical. The second option is to input a leaching constant greater than 0, which is the fraction of total chemical available for leaching annually, then a Kd value is estimated based on a leaching model that is included in the RESRAD-ECORISK code. The third option uses an empirical correlation between the distribution coefficient and the root-uptake transfer factor to calculate a Kd value. The last option uses the organic carbon content of the soil and the organic partitioning coefficient in the RESRAD-ECORISK database to calculate the Kd value.

The necessary meteorological data that are needed include precipitation rate, evapotranspiration coefficient, erosion rate, runoff coefficient, mass loading factor, and wind speed. The mass loading factor is an empirical parameter that specifies the ratio of air concentration of dust particles from resuspension to the soil concentration. The wind speed is used to calculate the dilution factor for volatile organic compounds that diffuse from the contaminated soil.

RESRAD-ECORISK OUTPUT

RESRAD-ECORISK generates a set of three tabular report files, a Summary Report file, an Environmental Media Concentration Report file, and a Detailed Report file. The Summary Report File lists (1) the transfer factors, chemical properties, and benchmark values used in the risk assessment, (2) the site-specific characterization data used for modeling contaminant fate and transport, (3) the uptake pathways used for each receptor in the current run, and (4) Chemical Abstract Service (CAS) numbers for the selected chemicals. These lists are followed by summaries of the ADD and EHQ values estimated for each pathway, contaminant, and receptor, and the estimated total EHQ for the user-selected time periods. The last item in the summary report is a list of the chemical soil guideline for each receptor modeled.

The Environmental Media Concentration Report file presents contaminant
CONCLUSIONS

RESRAD-ECORISK is a user-friendly computational tool for assessing ecological risks at chemically contaminated sites. The code may be used (1) as a screening tool to conduct a preliminary ecological risk assessment to determine if current levels of contamination pose a potential adverse risk to ecological resources, (2) to conduct a more detailed ecological risk assessment if site- and species-specific ecology and toxicology data are available, and (3) to develop preliminary soil guidelines that would reduce the risk to ecological receptors to acceptable levels.

RESRAD-ECORISK uses a methodology consistent with that applied in the RESRAD-CHEM code for modeling contaminant transport through different environmental media, thus permitting ecological and human health risks to be assessed with the same environmental media concentrations and fate and transport assumptions. As regulatory requirements increasingly emphasize the need for assessing ecological risk, RESRAD-ECORISK represents a useful software package that permits quick and comprehensive analyses in a timely, cost-effective manner.

REFERENCES


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