APPLYING RESRAD-CHEM FOR CHEMICAL RISK ASSESSMENT*

by

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ABSTRACT

RESRAD-CHEM is a multiple pathway analysis computer code to evaluate chemically contaminated sites; it was developed at Argonne National Laboratory for the U.S. Department of Energy. The code is designed to predict human health risks from exposure to hazardous chemicals and to derive cleanup criteria for chemically contaminated soils. It consists of environmental fate and transport models and is capable of predicting chemical concentrations over time in different environmental media. The methodology used in RESRAD-CHEM for exposure assessment and risk characterization follows the U.S. Environmental Protection Agency's guidance on Human Health Evaluation for Superfund. A user-friendly interface is incorporated for entering data, operating the code, and displaying results. RESRAD-CHEM is easy to use and is a powerful tool to assess chemical risk from environmental exposure.

ABOUT RESRAD-CHEM

Pathways Considered in RESRAD-CHEM

RESRAD-CHEM considers nine human exposure pathways: (1) inhalation of dust particles; (2) inhalation of volatile compounds diffusing from contaminated soil or volatilizing from household water use; (3) ingestion of plant food grown on-site and irrigated with water drawn from an on-site well or pond; (4) ingestion of meat from livestock fed with fodder grown on-site and watered from an on-site well or pond; (5) ingestion of milk from livestock fed with fodder grown on-site and watered from an on-site well or pond; (6) ingestion of soil; (7) ingestion of aquatic foods from a nearby pond; (8) ingestion of drinking water from an on-site well or pond; and (9) dermal absorption of chemicals from swimming, showering, and direct soil contact. Figure 1 is a schematic presentation of the exposure pathways.

Method of Analysis

The RESRAD-CHEM code analyzes risks to human health from exposure to hazardous chemicals in terms of hazard indexes (for noncarcinogenic effects) and cancer risks (for carcinogenic

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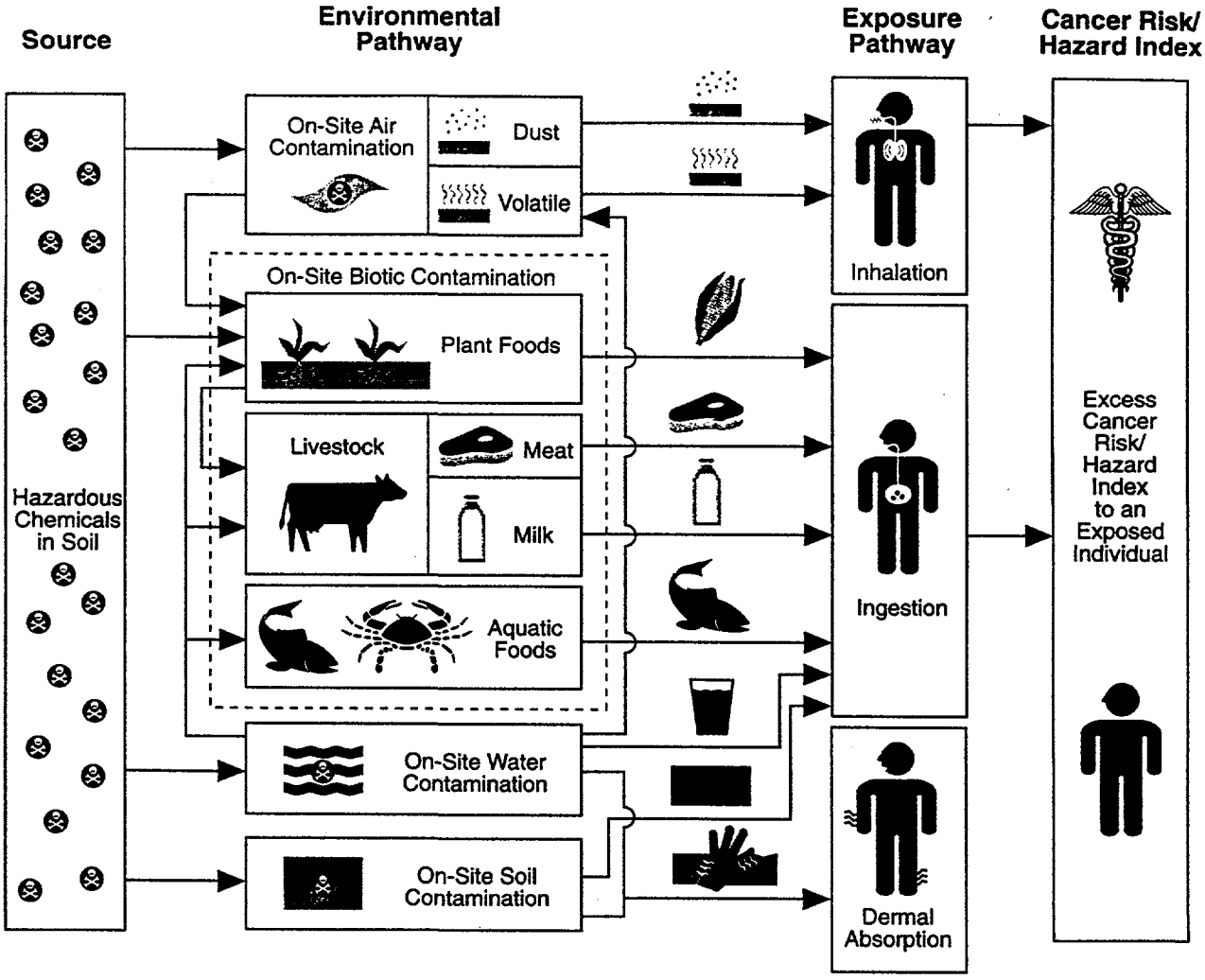

Figure 1 Schematic Presentation of the Exposure Pathways Considered by RESRAD-CHEM

effects). These methods are in accordance with the U.S. Environmental Protection Agency's (EPA's) guidance for evaluating human health [1]. The exposures and risks are calculated at user-specified times in the future, and RESRAD-CHEM calculates the maximum exposure and risk within the specified time frame. Soil cleanup criteria for individual chemicals are then derived on the basis of user-specified target risk levels (cancer risk for carcinogens and hazard index for noncarcinogens).

RESRAD-CHEM Features

A menu-driven interface was incorporated into RESRAD-CHEM from which the user can easily access the data input screens, run the RESRAD-CHEM calculations, and view the output. The system allows the user to suppress exposure pathways from the analysis and automatically blanks out nonapplicable input parameters.

One feature of the RESRAD-CHEM code facilitates sensitivity analyses on most input parameters. The results of the sensitivity analysis are output in a graphic form, which allows the user to easily see the influence of the input parameters and to prioritize efforts in data collection. The graphics option can also be used to generate publication-quality, hard-copy output on several devices, including dot-matrix printers, laser printers, and plotters.

RESRAD-CHEM Database

Currently, the RESRAD-CHEM database contains the 151 chemicals on the EPA's Target Compound List for Organics [2] and Target Analyte List for Inorganics [3]. More chemicals may be added later. RESRAD-CHEM allows users to modify the database of chemicals used in the calculations, thus providing considerable flexibility.

Information Generated by RESRAD-CHEM

After the calculations are complete, RESRAD-CHEM generates three report files: a summary report, a detailed report, and a concentration report. The summary report contains tables that present intake quantities, total cancer risks, and hazard indexes at different time periods for the different chemicals and pathways. Soil cleanup criteria for individual chemicals are also listed. The detailed report includes intermediate calculational results that help explain the mechanism of the transport process as described by the mathematical models and provides insight into the interaction among different exposure routes. The concentration report lists different environmental media concentrations by chemicals over the input time periods.

EXAMPLE

Contaminated Zone Characteristics and Exposure Scenario

A hypothetical site was contaminated by 1,1,1-trichloroethane, benzene, trichloroethene, and methylene chloride. The area of the contaminated zone was 10,000 m^2, and the thickness of the contaminated zone was 1 m. A layer of clean soil 0.5 m thick was placed on top of the contaminated zone. The groundwater table was 4 m below the bottom of the contaminated zone. A pond with a watershed area of 1,000,000 m^2 was located on-site, and a well with a screen depth of 10 m was located at the edge of the contaminated zone.

A residential scenario was assumed. The residents set up living on-site; grew plant foods (leafy and nonleafy vegetables, fruits, etc.); raised livestock for meat and milk; consumed aquatic foods caught from the on-site pond; swam in the pond for recreation; and used the well water for drinking, household use, and irrigation. It was further assumed that 50% of the consumed plant food was grown on-site, 50% of the meat and milk was from the livestock raised on-site, and 50% of the aquatic food was caught from the on-site pond. The exposed individual was assumed to spend 350 days a year on-site; while on-site, 33% of the time was spent outdoors. The total exposure duration was 30 years.

RESRAD-CHEM Calculation Results

All nine exposure pathways were selected when RESRAD-CHEM was used to analyze the potential risks incurred by the on-site resident. Except for the chemical concentrations in the contaminated zones (which were 1 mg/kg for each chemical), the RESRAD-CHEM default values were used in the analysis. The results showed that about 5% of 1,1,1-trichloroethane was left in the contaminated zone after 35 years. The times required to get to the same residual level for the other contaminants were as follows: for benzene, about 22 years; for methylene chloride, 4.5 years; and for trichloroethene, 31 years. Three mechanisms contribute to the depletion of source: leaching, volatilization, and erosion; leaching is the dominant factor. It took 25 years for 1,1,1-trichloroethane to reach the groundwater table, 15 years for benzene, 3 years for methylene chloride, and 22 years for trichloroethene.

Benzene is a class A human carcinogen. The unit risk for inhalation used in the RESRAD-CHEM database is 8.3×10^{-6} $(\mu g/m^3)^{-1}$, and the slope factor for ingestion is 2.9×10^{-2} $[mg/(kg\text{-}day)]^{-1}$. Methylene chloride is a class B2 human carcinogen, with a unit risk for inhalation of 4.7×10^{-7} $(\mu g/m^3)^{-1}$ and a slope factor for ingestion of 7.5×10^{-3} $[mg/(kg\text{-}day)]^{-1}$. Trichloroethene is classified as a C-B2 human carcinogen. In the database, the inhalation unit risk is 1.7×10^{-6} $(\mu g/m^3)^{-1}$, and the ingestion slope factor is 1.1×10^{-2} $[mg/(kg\text{-}day)]^{-1}$. According to the calculation results, the maximum cancer risk that the exposed individual received was 1.4×10^{-4} from benzene, occurring at 24 years. The maximum cancer risk that resulted from exposure to methylene chloride was 2.4×10^{-5} at 3.9 years. The maximum cancer risk caused by trichloroethene was 7.1×10^{-6} at 50 years. If the target cancer risk (maximum lifetime risk that the exposed individual received from the 30 years exposure duration) was set to 1.0×10^{-6}, then the cleanup criteria for soil concentrations would be 7.3×10^{-3} mg/kg for benzene, 4.1×10^{-2} mg/kg for methylene chloride, and 1.4×10^{-1} mg/kg for trichloroethene. Table 1 lists the maximum cancer risk components for the individual chemicals and pathways.

1,1,1-trichloroethane is not a human carcinogen; however, it will cause adverse health effects from chronic exposure. The inhalation reference concentration used in the RESRAD-CHEM database is 1.0 mg/m^3, and the ingestion reference dose is 9.0×10^{-2} mg/(kg-day). Methylene chloride can cause both carcinogenic and noncarcinogenic effects. In the database, the inhalation reference concentration is 3.0 mg/m^3, and the ingestion reference dose is 6.0×10^{-2} mg/(kg-day). According to the calculation results, the maximum hazard index (3.7×10^{-2}) occurred at 61 years for 1,1,1-trichloroethane. For methylene chloride, the maximum hazard index (9.2×10^{-2}) occurred at 3.9 years. The cleanup criterion was 27.2 mg/kg for 1,1,1-trichloroethane; for methylene chloride, it was 10.9 mg/kg, based on a target hazard index of 1 (i.e., the average hazard index resulting from 30 years exposure should not exceed 1). The hazard index components for individual chemicals and pathways are listed in Table 2.

Discussion

The lifetimes of 1,1,1-trichloroethane, benzene, methylene chloride, and trichloroethene in the soil phase were short because of the small soil/water distribution coefficients (*Kds*), which favor dissolution of chemicals in the pore-space water rather than adsorbing to the soil matrix. As a result, groundwater contamination was detected not long after the leaching started. From both

Table 1 Maximum Cancer Risk Components for Individual Chemicals and Pathways[a]

Pathway	Benzene	Methylene Chloride	Trichloroethene
Water Independent			
Dust	0	0	0
Volatile	2.25E-12	9.76E-12	2.45E-15
Plant	1.17E-07	4.62E-08	8.01E-14
Meat	9.30E-12	5.56E-13	1.16E-17
Milk	3.35E-12	2.12E-13	4.36E-18
Soil	0	0	0
Dermal	0	0	0
Water Dependent			
Volatile[b]	1.08E-04	1.16E-05	4.75E-06
Plant[b]	2.01E-06	1.20E-06	1.57E-07
Meat[b]	7.94E-10	6.02E-11	1.17E-10
Milk[b]	5.27E-10	4.19E-11	8.11E-11
Fish	2.99E-08	3.47E-09	3.84E-09
Water	2.26E-05	1.11E-05	1.83E-06
Dermal[b]	3.92E-06	4.32E-07	3.52E-07
Total[c]	1.37E-04	2.44E-05	7.09E-06

[a] Cancer risks were calculated at 24.1 years for benzene, 3.9 years for methylene chloride, and 49.6 years for trichloroethene.

[b] Cancer risks for water-dependent pathways result from groundwater irrigation, using or drinking groundwater, or body contact with surface water.

[c] Sum of all water-independent and -dependent pathways.

Tables 1 and 2, it can be seen that cancer risks or hazard indexes contributed by the water-dependent pathways are far more significant than those from the water-independent pathways. For the maximum cancer risks, inhalation of volatiles through household water use is the major contributor, followed by ingestion of water. For the maximum hazard indexes, the same conclusion holds for 1,1,1-trichloroethane. For methylene chloride, ingestion of drinking water causes more health concern than inhalation of volatiles. Use of a clean water source rather than an on-site well for drinking and household use would effectively reduce human health risks. For a contaminated site like this one, remediation efforts should be implemented promptly to avoid further spreading of the contaminants to the deeper soil.

Table 2 Maximum Hazard Index Components for Individual Chemicals and Pathways[a]

Pathway	1,1,1-Trichloroethane	Methylene Chloride
Water Independent		
Dust	0	0
Volatile	2.26E-09	1.61E-08
Plant	2.15E-05	2.40E-04
Meat	4.09E-09	2.88E-09
Milk	1.54E-09	1.10E-09
Soil	0	0
Dermal	0	0
Water Dependent		
Volatile[b]	1.92E-02	1.93E-02
Plant[b]	1.08E-03	6.22E-03
Meat[b]	1.07E-06	3.12E-07
Milk[b]	7.42E-07	2.17E-07
Fish	7.05E-06	1.80E-05
Water	1.27E-02	5.75E-02
Dermal[b]	2.64E-03	2.24E-03
Total[c]	3.57E-02	8.54E-02

[a] Hazard indexes were calculated at 60.9 years for 1,1,1-trichloroethane and 3.9 years for methylene chloride.

[b] Hazard indexes for water-dependent pathways result from groundwater irrigation, using or drinking groundwater, or body contact with surface water.

[c] Sum of all water-independent and -dependent pathways.

CONCLUSIONS

RESRAD-CHEM is a user-friendly tool for assessing chemical risks. The code incorporates such features as a graphic display and sensitivity analysis capability while providing sufficient flexibility to meet the users' needs for different situations. RESRAD-CHEM can be used to analyze the potential risks to human health from exposure to hazardous chemicals at a contaminated site. It can also be used to design a strategy to reduce the potential risks. The soil cleanup criteria that RESRAD-CHEM derives based on the target human health protection standards can be used to assist decision making for cleanup activities and to set remediation goals in the final design.

REFERENCES

[1] EPA (U.S. Environmental Protection Agency), *Risk Assessment Guidance for Superfund, Volume I: Human Health Evaluation Manual (Part A, Interim Final)*, Office of Emergency and Remedial Response, EPA/540/1-89/001,Washington, D.C. (December, 1989).

[2] EPA, *Contract Laboratory Program Statement of Work for Organics Analysis: Multimedia, Multi-Concentration,* Office of Emergency and Remedial Response, Document No. OLMO1.0, including revisions through OLMO1.8, Washington, D.C. (August, 1991).

[3] EPA, *Contract Laboratory Program Statement of Work for Inorganics Analysis: Multimedia, Multi-Concentration,* Office of Emergency and Remedial Response, Document No. ILMO2.0, including revision ILMO2.1, Washington, D.C. (September, 1991).