

MULTIMEDIA MODELING OF ENVIRONMENTAL RESTORATION RISKS AT ROCKY FLATS

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ABSTRACT

Computer-based multimedia models are key analytical tools for assessing potential exposure to environmental contaminants as the U.S. Department of Energy remediates its sites at the nuclear weapons complex. This study applies MEPAS, MMSOILS, and RESRAD to actual release site data from the 903 Pad Source Area within Operating Unit 2 at the Rocky Flats Environmental Technology Site using a common set of assumptions. The analysis compares the similarity of multimedia model output in terms of (1) prediction of transport, (2) determination of an individual's lifetime exposure, and (3) estimation of risk.

INTRODUCTION

Since their introduction in the late 1970s, multimedia models have been utilized to estimate exposure and risk from the transport and fate of chemical and radiological contaminants (1-2). The multimedia approach uses empirical expressions and analytical numerical solutions to estimate relationships between contaminant release rates, pollutant transport, intermedia fluxes, and subsequent exposure. Multimedia models typically combine estimates of human exposure via ingestion, inhalation, external radiation, and dermal absorption with measures of potency for cancer and non-cancer endpoints to assess risks (3-4). This paper, one of a series that describes the results of a multimedia model comparison study sponsored by the U.S. Department of Energy (DOE), examines the similarity of multimedia model output in terms of (1) prediction of transport, (2) determination of an individual's lifetime exposure, and (3) estimation of risk using actual site data and default parameters suggested by the individual model developers.

MULTIMEDIA MODEL AND CASE STUDY SELECTION

Three multimedia models (MEPAS, RESRAD, and MMSOILS) were selected for review for two reasons: (1) the sponsoring agency for the study requested these three models be reviewed due to DOE's technical and policymaking interest and (2) the models' ability to consider multiple pathways and to compute environmental transport across variable timeframes. MEPAS (Multimedia Environment Pollutant Assessment System), developed

by Pacific Northwest National Laboratory, MMSOILS, developed by the U.S. Environmental Protection Agency (EPA), and RESRAD (Residual Radiation), developed by Argonne National Laboratory, are multimedia environmental transport models that consider transport of contaminants in air, surface water, and groundwater, and bioaccumulation in plants and animals (5).

Briefly, MEPAS (6) is a highly automated multimedia model that has been applied to a wide range of potential environmental problems associated with DOE sites across the country. MEPAS was used in the Hanford Remedial Action Draft EIS, the Waste Isolation Pilot Plant Supplemental EIS, the Hanford Tank Waste EIS, and the Yucca Mountain EIS. In addition, MEPAS has been used by the state of Washington to develop cleanup standards. MEPAS has an extensive database of environmental and exposure parameters necessary for model calculations.

MMSOILS (7) was developed specifically to address risks at RCRA waste sites. MMSOILS was not designed to consider the transport of radionuclides, but it is possible to do so by considering radionuclides as inorganic contaminants with a first order decay. Such an approach does not allow for radioactive daughter ingrowth and thus can significantly underestimate exposures.

RESRAD (8) is a member of a family of specialized multimedia risk models in various stages of development that include: RESRAD-Chem, RESRAD Baseline, RESRAD Probabilistic, and RESRAD Recycle. RESRAD was developed primarily to assess decommission of radioactively-contaminated sites and because of this, points of groundwater exposure are limited to the facility boundary. This limits versatility in assessing multiple future exposure scenarios found in most risk assessments.

The reader who is interested in each model's technical formulations and detailed assumptions is referred to the manuals for MEPAS, MMSOILS, and RESRAD. Originally developed in the 1980's as screening tools to assist regulatory agencies in setting priorities and predicting risks for sites, the models basically assumed their present configuration in the early 1990's, although refinement and debugging is an ongoing effort. MEPAS V.3.1, MMSOILS version 4.0, and RESRAD version 5.62 and RESRAD-Chem (Beta version) were used for this study. Early drafts of the full report (9) on which this paper is based were provided to the model developers of the three models selected for review.

The model comparison effort utilized a case study approach to apply the three multimedia models to actual data based on real problems at DOE sites. The Rocky Flats Environmental Technology Site (RFETS) case study focuses on Operable Unit 2 (OU-2), which contains radioactive-contaminated oils and solvents, U-239 contaminated soils, liquid chemical waste disposal trenches, and an inactive Reactive Metal Destruction site. The RFETS case study includes exposures from contaminated surface soil and wind-blown dust. The RFETS case involves fairly routine exposure pathways in which multimedia models should produce similar results. An existing risk assessment and monitoring data were available as sources for site-specific input parameters. In the

absence of available site-specific input parameters, values recommended by model developers and the U.S. Environmental Protection Agency (EPA) were employed.

RFETS SITE CONCEPTUAL MODEL

Because the RFETS source areas for different sets of pathways and/or chemicals were not coincident, three conceptual site models are necessary:

VOC Conceptual Site Model. The VOC conceptual site model was developed to assess the potential risk associated with the use of groundwater contaminated with volatile organic chemicals (VOCs). The VOC source is restricted to a 3.6-ft-thick, 133,741-ft² area beneath an asphalt cover. The contaminants of potential concern (COPCs) included carbon tetrachloride, chloroform, tetrachloroethene, methylene chloride, trichloroethene, and 1,1-dichloroethene. The COPCs were assumed to have been released into the surface soil in 1958 and mean 1991-1992 values of measured soil and groundwater concentrations were used to estimate risk. Risk was determined based on a resident living on the down-gradient edge of the source term, exposed for 30 years to VOCs in soil and groundwater.

MEPAS and RESRAD CHEM recalculate soil-to-groundwater partition coefficients (K_d) to simulate movement of contaminants from the soil media into groundwater and ensure that estimated concentrations in groundwater are consistent with observed concentrations. MMSOILS does not recalculate K_d values based on observed concentrations. The MMSOILS user must select either measured soil concentrations or measured water concentrations. As a result, the estimated soil/groundwater concentrations may be different from measured concentrations. The multimedia models were not able to consider deterioration of the asphalt pad covering the contaminated soil; we assumed the asphalt pad would not be maintained and would deteriorate immediately, thereby allowing water to infiltrate the soil beneath it. This assumption is intended to provide conservative risk estimates. The edge of the asphalt pad in the direction of groundwater flow was selected as the groundwater receptor location.

A second potential pathway for exposure to VOCs is by inhalation. RESRAD uses a box model while MEPAS and MMSOILS apply dispersion models. For MEPAS and MMSOILS, air receptor locations were selected to coincide with points of greatest air concentration near the pad based on local atmospheric joint frequency data in the form of a Stability Array (STAR). Figure 1 summarizes the receptor locations and source area characteristics for the VOC conceptual site model.

To provide insight into how air receptor locations for the risk calculations were selected, we discuss the MMSOILS application. Since MMSOILS allows the user to specify up to 16 points at which atmospheric concentrations can be estimated, 16 equally spaced points were selected along a circle circumscribing the rectangular source. MMSOILS uses a dispersion model for estimation of although there are questions concerning the applicability of such a model when using receptor locations so close to the source. Of these, the two points with the greatest concentration were selected as exposure

concentration receptors (the maximum allowed per MMSOILS execution). By definition, the first point of the input file (in our case, that point associated with the greatest concentration) was used for PM10 and PM30 deposition to agricultural/cattle fields. The second point of the input file (in our case, that point associated with the second greatest concentration) was used as an off-site human exposure concentration.

Radionuclide Leaching Conceptual Site Model. The radionuclide leaching conceptual site model was developed to assess potential risks associated with the use of groundwater contaminated with plutonium 239/240. The conceptual site model considered the entire 10-acre 903 Pad Source Area. Because measured surface and subsurface plutonium concentrations differed significantly, we used a weighted mean of plutonium concentrations for the 3.6-ft-thick unsaturated contaminated zone. The down-gradient edge of the 10-acre site on the plume line was selected as the receptor location. Figure 2 summarizes the receptor locations and source area characteristics for the radionuclide leaching conceptual site model. As stated earlier, while RESRAD and MEPAS are designed to estimate risks for exposure to both radionuclides and their daughter products, MMSOILS does not simulate radioactive decay. Therefore, the estimates produced by MMSOILS reflect simple linear decay reactions of the radionuclides, which does not allow for radioactive daughter ingrowth and thus can underestimate exposures.

Radionuclide Dust Conceptual Site Model. The radionuclide dust conceptual site model was developed to address the potential risks associated with the inhalation of dust contaminated with plutonium 239/240. The conceptual site model considered the entire 10-acre 903 Pad Source Area and a 2-in.-thick contaminated soil zone beneath the concrete pad area. Mean surface soil plutonium concentrations were used as representative of the unsaturated, contaminated zone. Figure 3 summarizes the receptor locations and source area characteristics for the radionuclide dust conceptual site model.

MULTIMEDIA MODEL RESULTS

Detailed descriptions of the environmental setting, assessment scenario, and findings related to multimedia model differences for the RFETS case study are presented in the final report for the model comparison project ⁽⁹⁾. Provided here is a summary description of the major findings obtained by applying the multimedia models to the conceptual site models organized by the following topics: exposure pathways; contaminants of concern; risk estimates; and hazard indices. We also provide the results of the original Rocky Flats risk assessment for OU-2 (hereafter, OU-2 risk assessment) as a reference point for comparison (10).

Exposure Pathways. Table I indicates, as was true for the RFETS risk assessment, that MEPAS and RESRAD identified two groundwater pathways, drinking water ingestion and shower vapor inhalation, as the pathways with the highest excess lifetime cancer risk for a hypothetical on-site residential receptor. Two soil pathways, soil ingestion and resuspended dust inhalation, also are significant from an excess lifetime cancer risk standpoint. The differences in the MEPAS, RESRAD and RFETS risk estimates are

generally greater than two orders of magnitude for secondary pathways. The formulation and parameterization of the food chain components of the three multimedia models are similar. Table I indicates that risk for plant intake, meat ingestion, and milk ingestion are within 2 orders of magnitude for all three models. These variations result from differences in predicted groundwater concentrations that are used to compute concentrations in food.

Contaminants of Concern. Table I reveals that MEPAS and RESRAD assign similar risks to carbon tetrachloride, chloroform, tetrachloroethylene, and plutonium 239/240. Plutonium 239/240 was the only contaminant of concern identified by MMSOILS.

Risk Estimates. The MEPAS and RESRAD model simulations generally are consistent with the OU-2 risk assessment in terms of the magnitude of the risk. It is important to note that what we term “RESRAD” simulations are actually RESRAD simulations for the Radionuclide Leaching and Radionuclide Dust conceptual site models, combined with RESRAD Chem simulations for the VOC conceptual site model. Some of the discrepancy between MEPAS and RESRAD is due to the use of different reference dose levels (RfDs) in the absence of recommended values within the EPA IRIS database. MEPAS uses representative inhalation RfDs for the chlorinated volatile organic constituents while RESRAD uses zero as a RfD for chlorinated volatile organic constituents in the absence of established values.

The MMSOILS risk estimates differ substantially from those produced by MEPAS and RESRAD as well as the original Rocky Flats risk estimates (see Table I). A portion of the discrepancy stems from differences in how the three models predict groundwater concentrations. When both measured soil and groundwater concentrations are available, MEPAS and RESRAD permit changing model parameters to assure that predicted concentrations resulting from the initial placement of waste are comparable with measured concentrations. For example, RESRAD offers four options to correct for an inconsistency occurring when predicted groundwater concentrations at a future time do not correspond to measured groundwater concentrations. The user may adjust the soil-water partitioning coefficients, the time since contaminant placement, the concentration of contaminants in groundwater, or a combination of these options to produce groundwater concentrations that are comparable with those measured.

Although MMSOILS can use measured groundwater concentrations to make predictions, if this option is used, the model does not account for additions to the saturated zone that could cause the concentrations to increase. Thus, predicted future concentrations tend to be low. We utilized two different approaches in an effort to improve the accuracy of MMSOILS predictions. First, MMSOILS was run from 1991 forward using 1991-1992 groundwater concentrations as initial conditions. When adjusted K_d values from MEPAS and RESRAD were used as input parameters for MMSOILS, this failed to produce groundwater concentrations comparable to those measured subsequent to 1991-92 because initializing MMSOILS for 1991 does not account for leaching that occurred in the 33 years prior to 1991. The second approach, essentially inverse parameter estimation, involved beginning the model application 33 years prior to 1991 when the waste was first

Table I. Risks by exposure pathway and contaminant for each multimedia model

<i>Exposure Pathway</i>	<i>RFET</i>	<i>MEPAS</i>	<i>RESRAD & RESRAD CHEM</i>	<i>MMSOILS^a</i>
Drinking Water Ingestion	1.0E-02 ^b	2.2E-03	1.9E-03 ^b	8.7E-08
Shower Water Ingestion		1.1E-05		
Leafy Vegetables Ingestion	6.4E-07	5.9E-05		4.2E-05
Other Vegetable Ingestion	5.1E-06	3.9E-05		1.1E-09
Plant total ^c	5.7E-06	9.9E-05	2.8E-06	4.2E-05
Meat Ingestion		3.6E-09	1.8E-06	2.0E-06
Milk Ingestion		3.1E-09	8.8E-08	3.2E-07
Soil Ingestion	1.4E-04	8.4E-04	1.4E-05	1.6E-02
Soil Dermal Absorption	2.2E-09	5.1E-07	4.3E-17	7.3E-07
Showering Dermal Absorption		7.5E-04	3.3E-04	1.5E-08
Shower Vapor Inhalation	4.5E-03	7.9E-03	2.9E-03	
Air Volatile Inhalation	1.1E-09	1.9E-07	1.3E-12	
Resuspended Dust Inhalation	3.1E-05	2.0E-03	3.3E-06	
Total Air ^d	3.1E-05	2.0E-03	3.3E-06	3.E-04
Soil External	1.0E-05	2.6E-05		
Radon Inhalation			2.9E-18	
<i>Contaminant</i>	<i>MEPAS</i>	<i>RESRAD & RESRAD CHEM</i>	<i>MMSOILS^a</i>	
Carbon Tetrachloride	3.4E-03	2.5E-03	2.9E-08	
Chloroform	3.1E-03	1.6E-03	2.9E-08	
Tetrachloroethylene	2.7E-03		1.3E-08	
Dichloromethane	2.1E-04	8.4E-05	7.4E-07	
Trichloroethylene	7.8E-04		1.8E-08	
1,1 Dichloroethylene	3.0E-05	5.6E-04	1.1E-09	
Pu 239/240	3.6E-03	4.1E-04	1.7E-02	

a. MMSOILS was incompatible with the defined conceptual site model and did not use measured groundwater contaminant concentrations to calculate risk. Instead, MMSOILS calculated groundwater concentration of contaminants from measured soil concentrations. The calculated concentrations do not reflect the accumulation of contaminants in groundwater since their place placement in 1958. Instead, leaching begins in 1991/92 and results in lower than observed concentrations of contaminants in groundwater and lower risk values as a result.

b. Risk from ingestion of groundwater used for drinking and washing plant total (risk) is the sum of the risk from leafy vegetable ingestion and other vegetable ingestion air total (risk) is the sum of risk from volatile and resuspended dust inhalation.

placed in the ground. Because MMSOILS does not allow automated use of the 1991-92 groundwater concentrations to optimize on K_{oc} and soil concentrations, the input parameters for K_{oc} and soil concentration were adjusted so that, after 33 years of leaching, a groundwater concentration was computed to be nearly that of the observed

groundwater concentration. This "calibration" effort led to a groundwater concentration of 0.6202 mg/L for carbon tetrachloride (the measured CCl_4 groundwater concentration was 0.720 mg/L), which was then used by MMSOILS in computing a risk value of $9.9\text{E-}04$, a value comparable to the CCl_4 risk computed by the other two models. While this design feature of MMSOILS is not a major problem, it impacts the time required to apply the model and requires the model user to have an understanding of how different multimedia models make use of such input parameters as points and intervals in time, intervals over which risk is computed, time of placement of initial waste inventory, and time of measurement. A thorough understanding of the use of these parameters is required for successful conceptual site model development and application for risk assessment.

Hazard Indices. Examination of the hazard indices in Table II reveals patterns similar to those for excess lifetime cancer risk estimates (Table I), although the hazard indices exhibit greater variability. The hazard quotients (the sum of the individual hazard indices) estimated by MEPAS, RESRAD, and the OU-2 risk assessment exceed one, indicating that a hypothetical on-site resident potentially would be exposed to toxic constituent levels. Also, as was the case with excess lifetime carcinogenic risks, the pathways of greatest concern are drinking water ingestion and shower vapor inhalation.

CONCLUSIONS

Our multimedia model comparison study demonstrates that MEPAS, MMSOILS, and RESRAD can be used successfully to identify exposure pathways and estimate risk. All three multimedia models had sufficient flexibility to be adapted to use at RFETS, although their relative compatibility with actual site data varied (e.g., RESRAD requires soil concentrations which can be problematic when only groundwater data exist). When applied to real DOE sites using actual data, the models achieved agreement on major exposure pathways and contaminant concentrations exceeding two orders of magnitude due largely to differences in transport and fate. This points to the need for order-of-magnitude analysis to avoid model misuse.

The primary benefit of the screening-level capability inherent in multimedia models is the identification of contaminants and pathways making the largest contributions to overall risk associated with environmental remediation. To do this well, a multimedia model needs the capacity to reflect realistically site conditions. This involves the ability to incorporate generalized assumptions about the amount and location of contaminants, spatial and temporal distributions of potential receptors, and exposure pathways. Because multimedia models necessarily simplify empirical reality, applying the multimedia models to real data requires skill on the part of the risk assessor coupled with understanding of the environmental setting and parameterization of the models to avoid introducing substantial estimation error. Plausible estimates of risks by major pathways using actual site data can only be derived when the multimedia model is compatible with the conceptual site model.

Table II. Hazard indices by exposure pathway and contaminant for each multimedia model

<i>Exposure Pathway</i>	<i>RFET Estimate</i>	<i>MEPAS</i>	<i>RESRAD CHEM</i>	<i>MMSOILS^a</i>
Drinking Water Ingestion	1.6E+02 ^b	2.4E+01	3.1E+01 ^b	1.6E-03
Shower Water Ingestion		1.2E-01		
Leafy Vegetables Ingestion	1.9E-04	1.5E-02		1.4E-05
Other Vegetable Ingestion	2.2E-03	9.1E-02		2.2E-05
Plant total ^c	2.4E-03	1.1E-01	4.2E-06	3.6E-05
Meat Ingestion		3.2E-05	9.3E-04	5.5E-08
Milk Ingestion		9.6E-06	1.4E-03	3.3E-07
Soil Ingestion	5.8E-05	2.3E-04	1.5E-08	3.2E-10
Soil Dermal Absorption	1.9E-05	1.4E-02	2.6E-11	2.3E-09
Showering Dermal Absorption		8.6E+00	8.1E+00	2.5E-04
Shower Vapor Inhalation	5.0E-02	1.7E+02		
Air Volatile Inhalation	2.8E-09	1.8E-06		
Resuspended Dust Inhalation		4.7E-06		
Air Total ^d	2.8E-09	6.4E-06		5.1E-09
<i>Contaminant</i>	<i>MEPAS</i>	<i>RESRAD CHEM</i>	<i>MMSOILS^a</i>	
Carbon Tetrachloride	1.8E+02	3.2E+01	7.4E-04	
Chloroform	1.1E+01	3.4E+00	1.1E-03	
Tetrachloroethylene	6.9E+00	9.9E-02	5.7E-05	
Dichloromethane	3.2E+00	2.9E-01	2.7E-05	
Trichloroethylene				
1,1 Dichloroethylene	8.4E-01	1.5E-01	7.7E-09	

a. MMSOILS was incompatible with the defined conceptual site model and did not use measured groundwater contaminant concentrations to calculate risk. Instead, MMSOILS calculated groundwater concentration of contaminants from measured soil concentrations. The calculated concentrations do not reflect the accumulation of contaminants in groundwater since their place placement in 1958. Instead, leaching begins in 1991/92 and results in lower than observed concentrations of contaminants in groundwater and lower risk values as a result.

b. risk from ingestion of groundwater used for drinking and washing

c. plant total (risk) is the sum of the risk from leafy vegetable ingestion and other vegetable ingestion

d. air total (risk) is the sum of risk from volatile and resuspended dust inhalation. MMSOILS does not report these exposure pathways independently.

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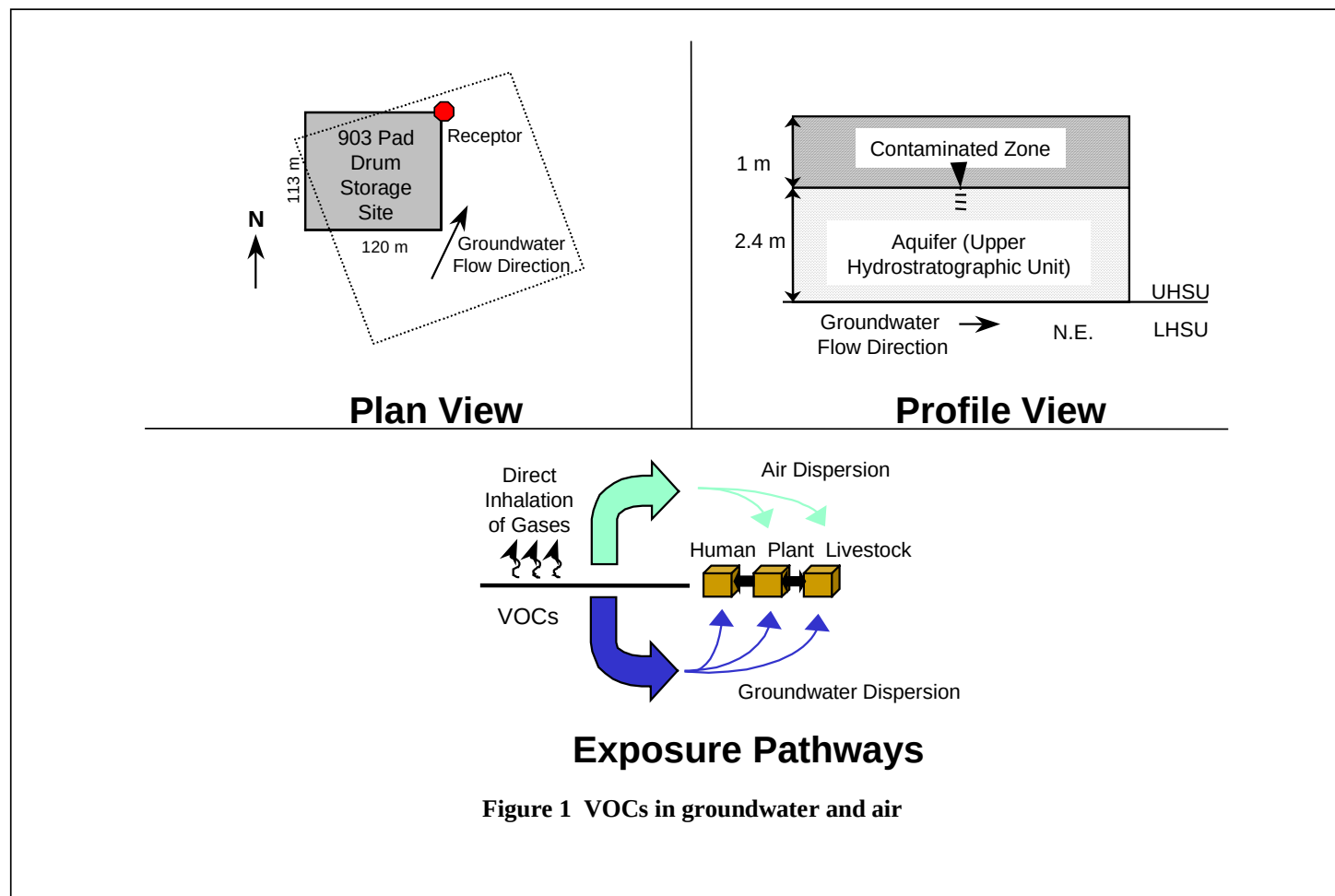
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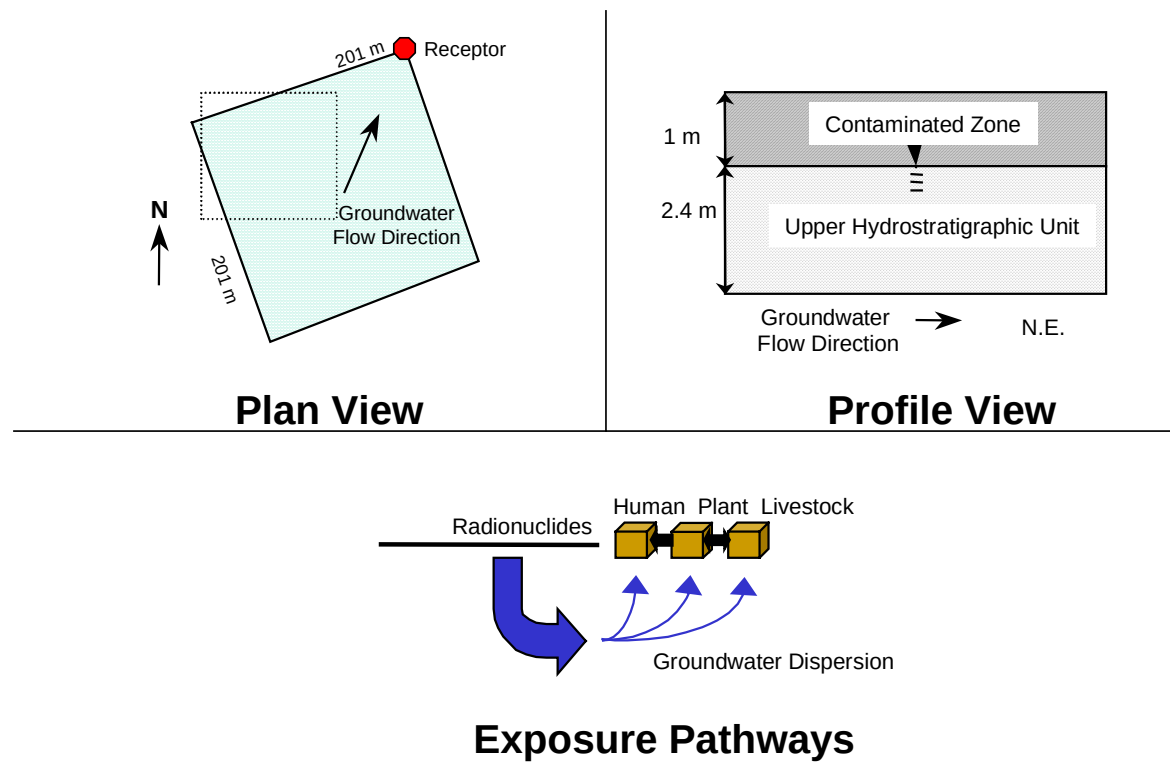


Figure 2 Radionuclides in groundwater

