

Integrated Water Resources Management in the Lower Jordan Rift Valley

Sustainable Management of Available Water Resources with Innovative Technologies



Deliverable D604 Platform for risk assessment

Evaluation of RBCA-based software platforms and associated modeling tools

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Environmental & Water Resources Engineering – EWRE Ltd.

April 2013

Funded by



Federal Ministry
of Education
and Research

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Key words:

Risk Based Corrective Action, Groundwater, Vadose Zone, Computer Software, Models

Funded by the German Federal Ministry of Education and Research (BMBF):

FKZ 02WM0801

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1. Introduction

In the frame of SMART substantial resources are devoted to the determination of areas vulnerable to pollution and to the delineation of protection zones. While the vulnerability concept is inherently related to the area and to the potential pollution sources within it, the concept of the definition of meaningful protection zones has to rely on some estimation of risks. In general terms a risk can be quantitatively defined as the product of the probability of an event of concern by the magnitude of its impact. Therefore, the risk concept requires a clear definition of what is a risk that needs to be addressed and tools for quantifying its impact.

An abundant literature is available regarding risk assessment methodologies and it is beyond the scope of this deliverable to review it in a comprehensive way but rather concentrated on a widely used and accepted platform for risk assessment. These are the RBCA (Risk Based Corrective Action, "Rebeca") methodology. This methodology is based on the assumption that risk calculation is based on the S-P-R (sources – pathways – Receptors) paradigm, claiming that a risk exists when there is a pathway that connects a source of pollution to a receptor (a compartment that is sensitive to the pollution under scrutiny). The RBCA methodology has been formulated in ASTM publications and there exist many specific implementations in most of the industrialized countries (The USA, Canada, many countries in Europe). There are also generic tools for site specific RBCA implementation.

The purpose of this deliverable is therefore to evaluate some of the more widely used software platforms in the Risk-Based Corrective Action, to be denoted hereafter as RBCA, process.

The deliverable comprises of five sections:

1. Introduction to the RBCA methodology: a summary of the RBCA terminology and process.
2. Software platforms: a description of seven commonly used computer programs and associated modeling tools that were evaluated.
3. Scenarios: a description of the three scenarios used in this work to evaluate the programs.
4. Results and discussion: a comparison of the target levels and risk levels calculated by the evaluated programs.
5. General data: technical data of the programs such as prices, availability of technical support and projects in which the programs were used.

2. The Risk-Based Corrective Action (RBCA) methodology

The **RBCA** is a consistent decision-making process for the management of remedial response of contaminated sites. This process includes a tiered (hierarchical) approach that integrates site assessment and response actions with human health and ecological risk assessment to determine the need for remedial action and to tailor corrective action activities to site specific conditions and risk.

Risk assessment is the analysis of the potential for adverse effects on receptors (Humans, ecological receptors and habitats) caused by chemicals of concern from a site. The risk assessment activities are the basis for the development of corrective action.

Calculating risk is called the “forward calculation” whereas calculating clean-up levels is called the “back calculation”.

For carcinogenic effects, risk is quantified using Individual Excess Lifetime Cancer Risk (IELCR) and for non-carcinogenic effects, the risk is quantified using a Hazard Quotient (HQ) or a Hazards Index (HI).

The risk levels define whether a contaminated site poses a risk to human beings and if a target level for remediation needs to be calculated for the site.

According to the IRBCA technical guide, for Tier 2 the risk threshold for hazard quotient (HQ) is 1.0 and for cancer risk (IECLR) is 1×10^{-5} for the sum of all exposure routes or 1×10^{-6} for a single exposure route (risk levels are non-dimension indicators). In other words, if the risk level is below these values, there is no need for the determination of target levels for the site.

2.1 Terminology

The following definitions are from the IRBCA technical guide:

- **Chemical(s) of Concern:** Specific contaminants that are identified for quantitative evaluation in the risk assessment process and are deemed to be related to anthropogenic activities at the site.
- **Forward mode calculation:** The calculation of risk from input or estimated receptor point concentrations and receptor input parameters (see [Figure 2.1](#)). This option requires applicable source zone chemical of concern (COC) concentrations to be entered for affected soil and/or groundwater.
- **Backward mode calculation:** The calculation of “allowable” source concentrations for each complete exposure pathway identified in the exposure model and for each COC (see [Figure 2.1](#)), based on target risks or target concentrations (e.g. Israeli Drinking Water Standards) determined by the user. The clean-up levels (also refer to as target levels) represent source and/or receptor point concentrations for the chemicals of concern such that the risk levels

are not exceeded for the scenario outlined. This option does not require source zone COC concentrations.

- **Site specific target levels (SSTLs):** Allowable COC concentration in source medium. SSTLs address actual site-specific exposure conditions and situations where the point of exposure (POE) may be located at some distance away from the source. For each complete exposure pathway, cleanup levels for the source medium can be back-calculated from safe exposure levels at the POE.
- **Site specific conditions:** A general description of a site's chemical, physical or biological characteristics that relate to potential exposures to receptors.
- **Point of exposure (POE):** The location where chemicals enter the human body or the body of the ecological receptor or its habitat.
- **Exposure Pathway:** Physical migration of contaminants from sources to the receptor. An exposure pathway describes a unique mechanism by which an individual or population (human and ecological receptor or ecological habitat) is exposed to a COC and its byproducts originating from a site. Each exposure pathway includes a source or release from a source, a point of exposure, an exposure route and a receptor. If the exposure point is distant from the source, a transport/exposure medium (for example, air) or media also is included.
- **Exposure Route:** The manner in which a COC comes in contact with an organism (for example, ingestion, inhalation, and dermal contact).
- **Hazard Quotients:** The ratio of the dose to the reference dose for that chemical.
- **Hazard Index:** The sum of two or more hazard quotients (HQ) for multiple chemical(s) of concern or multiple exposure pathways, or both and can be used to predict the non-cancer risk of simultaneous exposure of a receptor to several chemicals.
- **Incremental Carcinogenic Risk Levels:** The potential for incremental carcinogenic human health effects due to exposure to the COC.

2.2 The three-tiered approach

RBCA process employs a tiered approach to derivation of risk-based soil and groundwater cleanup goals. In each tier, risk-based concentration limits are derived for relevant exposure pathways, receptors, and constituents of concern and compared to measured source media concentrations. Source media exceeding these target levels will require either further investigation or remedial action in the timeframe necessary to control exposure.

Tier 1 Evaluation - general site assessment information: A risk based analysis utilizing non-site-specific corrective action goals for complete and potentially complete direct and indirect human exposure, ecological receptors and habitats. It is based on a conservative assumption and methodologies to estimate the non-site-specific values. The assumption is that the receptor and source are located in the same vicinity. The

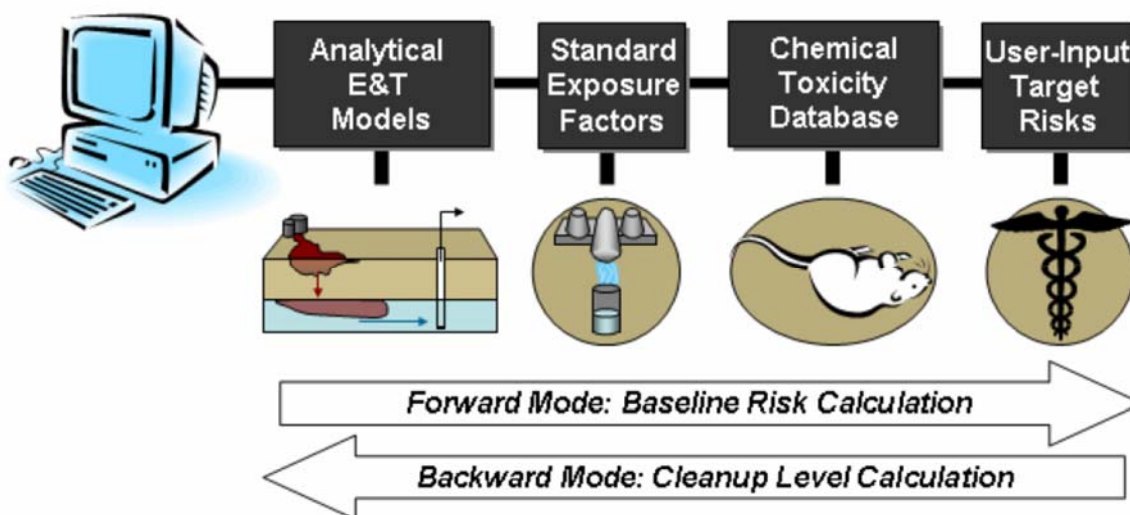
corrective action goals are compared to site conditions to determine if further corrective action is warranted.

Tier 2 Evaluation – specific site assessment information: A risk based analysis that involves an incremental refinement of the Tier 1, in order to develop site-specific corrective action goals. Here, the reasonable maximum site-specific impact is evaluated through the use of site-specific characterization and monitoring data, conservative projections of expected levels of contaminants after treatment and reasonable maximum exposure scenarios. This information is used to set conservative corrective action objectives that are protective of human health and the environment. The corrective action goals are compared to site conditions to determine if further corrective action is warranted.

Tier 3 Evaluation – advanced specific site assessment information: A risk based analysis that involves a significant incremental effort over the Tier 2, in order to develop site-specific corrective action goals. It focuses completely on the site-specific conditions. More sophisticated mathematical descriptions of fate and transport phenomena are used and descriptions of the range of possible exposures/risks are generated. At this level of complexity, site specific risk assessment models may be developed. Due to the costs involved, this analysis is suited to only large sites.

It is important to note that the goal of all tiers is to achieve similar levels of protection. The difference is that, in moving to higher tiers, more efficient and cost-effective corrective action result because the conservative assumptions of earlier tiers are replaced with more realistic site-specific assumptions. Additional site assessment data may be required as sites move to higher tiers. The results of all of the completed tiers are compiled into one evaluation report.

Figure 2.1: **Forward and backward calculation modes**



3. RBCA-based software platforms

3.1 Models and solution techniques

The Standard Guide for Risk-Based Corrective Action (ASTM E2081, 2010) defines mathematical models (in the context of RBCA) as “any of the calculations that are used in the various steps of the RBCA process to determine corrective action goals. These models are most typically associated with assessing the fate and transport of chemicals in the environment. Models are also used to estimate chemical uptake that result from environmental exposure and to interpret, interpolate, extrapolate and assess the consistency of site characterization data, historical monitoring data and toxicological information”.

Models (or solution techniques) are categorized as analytical, numerical, or a hybrid of the two:

- Analytical models: The governing equation is solved directly or by means of a simplified solution to the governing equation.
- Numerical models: Use techniques such as finite difference or finite element methods to solve the governing equation.

Objectives of modeling should be defined before model selection begins for it is possible that a simple model will be adequate to provide the desired information. The complexity of selected models should balance the quantity and quality of available input data (or of data which can be obtained easily) with the desired model output (Foster Wheeler Environmental Corporation, 1998).

3.1.1 Analytical solutions

Analytical solutions are based on mathematical functions that are or have the potential to be exact solutions of the transport equation. Analytical solutions of the transport equation:

- Unable to simulate heterogeneous formations;
- Requires the assumption of one-dimensional flow;
- Only represents uniform flow;;
- Includes transport by advection in the direction of flow only;
- Unable to represent irregular boundaries.

3.1.2 Numerical solutions

Numerical models are based on approximations that are formulated over necessarily small parts of the simulation domain. The two most common numerical methods are finite difference and finite element, both of which require a grid to be placed over the domain. This provides a way to identify these models—if there is a gridded domain then the model is most likely to be a numerical model; otherwise the model is analytical (Weaver et al., 2005).

3.2 Description of software platforms and models

For the purpose of this deliverable, seven commonly-used computer software packages were evaluated. The packages are divided in two:

1. Programs which model migration of the constituent: VLEACH, BIOSCREEN, Tier2 Analyzer.
2. Programs which combine both migration models and risk and target levels assessments: RBCA Tool kit, RISC5, Johnson & Ettinger (EPA) and IRBCA¹.

A short description of the main features of each package is shown below.

3.2.1 VLEACH

VLEACH, A One-Dimensional Finite Difference Vadose Zone Leaching Model, is a computer code for estimating the impact due to the mobilization and migration of a sorbed organic contaminant located in the vadose zone on the underlying groundwater resource.

The model was initially developed by CH₂M Hill for the U.S. Environmental Protection Agency, Region IX in 1990 (Ravi et al., 1997).

3.2.1.1 The model

The model describes the movement of an organic contaminant within and between three different phases: (1) as a solute dissolved in water, (2) as a gas in the vapor phase, and (3) as an adsorbed compound in the solid phase. Equilibration between the phases occurs according to distribution coefficients defined by the user. VLEACH simulates vertical transport by advection in the liquid phase and by gaseous diffusion in the vapor phase. During each time step the migration of the contaminant within and between cells is calculated:

1. Step 1 - VLEACH calculates the equilibrium distribution of contaminant mass between the liquid, gas, and sorbed phases.
2. Step 2 - Liquid advective transport is calculated based on values defined by the user for infiltration and soil water content.
3. Step 3 - Diffusive transport of gas is calculated: The contaminant in the vapor phase migrates into or out of adjacent cells based on the calculated concentration gradients that exist between adjacent cells.
4. Step 4 - Recalculate total mass in each cell: After the mass is exchanged between the cells, the total mass in each cell is recalculated and re-equilibrated between the different phases.

¹ The Johnson & Ettinger and the IRBCA programs have limited capabilities for modeling transport of COC.

These steps are conducted for each time step, and each polygon is simulated independently. At the end of the model simulation, the results from each polygon are compiled to determine an overall area weighted groundwater impact for the entire modeled area (Varadhan et al.).

It should be noted that VLEACH uses an expression of the Millington's equation for gaseous diffusion coefficient in air-filled pore spaces, in which the exponent was changed from 10/3 (as used in other models examined in this study) to 7/3:

$$\frac{D_p}{D_{air}} = \frac{(\psi_a)^{7/3}}{\psi^2}$$

3.2.1.2 Output

- Equilibrium distribution of constituent mass between liquid, gas, and sorbed phases.
- Area-weighted groundwater impact for modeled area.

3.2.1.3 Assumptions and limitations

1. The vadose zone is in a steady-state condition with respect to water movement.
2. Homogenous soil conditions within polygon.
3. Instantaneous equilibrium occurs between the three phases in each vertical cell.
4. A depleting source of contamination.
5. Assumes volatilization is either completely unimpeded or completely restricted.
6. Does not incorporate degradation or in situ production.
7. Does not account for dispersion.
8. Non-aqueous phase liquid or variable density flow is not considered.

3.2.1.4 Sensitive input parameters

1. Organic carbon distribution coefficient
2. Effective porosity
3. Soil organic carbon content
4. Initial contaminant concentration

3.2.2 BIOSCREEN

An analytical groundwater model which simulates remediation through natural attenuation (RNA) of dissolved hydrocarbons at petroleum fuel release sites. The software is programmed in the Microsoft Excel spreadsheet environment and based on the Domenico analytical solute transport model. Contaminant transport is simulated under 1-D horizontal groundwater flow (Cecan et al., 2010). It has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions (Newell et al., 1997).

3.2.2.1 The Domenico analytical solute transport model

The Domenico analytical model, used by BIOSCREEN (and also by RBCA Tool Kit) is designed for the multidimensional transport of a decaying contaminant species:

$$C(x, t) = \frac{C_0}{2} \exp \left[\frac{x}{2\alpha_x} \left(1 - \sqrt{1 + \frac{4\lambda\alpha_x}{v}} \right) \right] \times \operatorname{erfc} \left[\frac{x - vt\sqrt{1 + \frac{4\lambda\alpha_x}{v}}}{2\sqrt{\alpha_x vt}} \right] \operatorname{erf} \left[\frac{Y}{2\sqrt{\alpha_y x}} \right]$$

Where:

C_0 = the initial concentration

α_x = longitudinal dispersivity

α_y = transverse dispersivity

k = the rate of biodegradation

t = time

x = distance from source

v = the retarded velocity ($v = v_s/R$, R is the retardation factor and v_s is seepage velocity)

Y = the width of the source.

The key assumptions in the Domenico model are:

1. The aquifer and flow field are homogeneous and isotropic.
2. The groundwater velocity is fast enough that molecular diffusion in the dispersion terms can be ignored (is not appropriate for simulation of transport through low permeability media).
3. The source contaminant concentration remains constant through time.
4. Adsorption is a reversible process represented by a linear isotherm.

The key limitations to the Domenico model are:

1. The model should not be applied where pumping systems create a complicated flow field.
2. The model should not be applied where vertical flow gradients affect contaminant transport.
3. The model should not be applied where hydrogeologic conditions change dramatically over the simulation domain.
4. Domenico-based models are approximate analytical solutions of the advective-dispersive solute transport equation; therefore, they could generate an error for a

given set of input parameters when compared with the exact solutions. The error is largely sensitive to high values of longitudinal dispersivity (CSMoS home page).

The most important modifications to the original Domenico model are:

1. The addition of "layer cake" source terms where three Domenico models are superimposed one on top of another to yield the 5-source term used in BIOSCREEN.
2. Adaptation to provide 3 different model types: i) Solute transport without decay; ii) Solute transport with biodegradation modeled as a first-order decay process (simple, lumped-parameter approach); iii) Solute transport with biodegradation modeled as an "instantaneous" biodegradation reaction.
3. The addition of a declining source concentration term in order to overcome the basic assumption of an infinite source in the Domenico model.

3.2.2.2 Output

The program output shows concentrations along the centerline (for all three kinetic models at the same time) or as an array (one kinetic model at a time). Note that the results are all for the time entered in the "Simulation Time" box.

Centerline Output

The centerline output screen shows the average concentration at the top of the saturated zone ($Z=0$) along the centerline of the plume ($Y=0$).

Array Output

A 3-D graphic shows results on a 10-point-long by 5-point-wide grid. An approximate mass balance is presented on the array output screen.

BIOSCREEN does not produce a point of compliance report (which presents a graphical representation of constituent concentrations over time at a specific point – $x(t)$) and as such the software has to be run repeatedly until sufficient data is produced to generate a point of compliance report (Cecan et al., 2010).

3.2.2.3 Sensitive input parameters

1. Source area contaminant concentrations,
2. Saturated hydraulic conductivity,
3. Distance along the center line from down gradient edge of dissolved plume source zone.

3.2.3 RBCA Tier2 Analyzer

Tier2 analyzer is a software package which consists of 2-D groundwater flow and solute transport codes and an initial-condition plume generator.

3.2.3.1 Model

The analytical flow model allows the incorporation of multiple boundary conditions representing various combinations of extraction and injection wells, no-flow boundaries, leaky-type (semi-pervious layer) boundaries such as rivers and lakes with complex geometries, and regional hydraulic gradients. The model is based on the

superposition of Dupuit-Forchheimer solutions for flow to one or more wells and the effects of a regional hydraulic gradient.

The contaminant transport incorporates the physics of multi-site, rate-limited (or “slow”) partitioning of chemical mass between soil and groundwater. Either equilibrium or nonequilibrium partitioning may be selected for the single-constituent, PCE decay chain, or BTEX biodegradation options. The transport code also simulates advection, dispersion, retardation (equilibrium sorption), dilution by rainwater infiltration, and biodegradation or decay as a first-order process. The solution technique utilized to solve the governing solute transport equation is the Eulerian-Lagrangian method, which practically eliminates numerical dispersion (Cosler et al.,).

The initial-condition plume model provides the user with the optional capability of generating physically realistic contaminant plumes. The foundation of the initial-condition plume generator is the analytical solution for the two-dimensional concentration distribution within a single Gaussian puff.

3.2.3.2 Output

The RBCA Tier 2 Analyzer includes a selection of graphical capabilities for visualizing and interpreting the modeling results. Output graphics include:

1. Contouring and color shading of head and concentration values.
2. Flow path lines and velocity vectors.
3. Concentration time-series graphs for any location in the model domain.
4. Animation of flow path lines and contaminant plumes.

3.2.4 RISC5

The Risk Integrated Software for Clean-ups (RISC) was developed by BP and is a Windows based package for the multi-media risk assessment of contaminated land. It contains contaminant fate and transport models for predicting exposure point concentrations, a wide range of exposure pathways and a large chemical database with toxicological, fate and transport, and regulatory standards. The fate and transport models included in the RISC5 software are described hereinafter.

3.2.4.1 Vadose zone model

A 1-D advective - dispersive solute transport equation (van Genuchten & Alves, 1982).

The output of the model includes:

1. Mass flux at the water table as a function of time;
2. Cumulative mass loading to GW;
3. Leachate concentration at WT

Assumptions and limitations:

1. Does not simulate the movement of NAPL.
2. The vadose zone is considered to be homogeneous and uniform below the source.
3. The hydraulic conductivity is calculated as a function of moisture content, however, this derived moisture content is assumed to be constant for the entire depth of the soil column.
4. The contaminant source has a uniform concentration across the user-specified source volume.
5. Water table fluctuations are not considered. The depth to the aquifer is considered fixed.

6. Assumes a finite mass source.

3.2.4.2 Saturated zone model (DISSOLVED-PHASE TRANSPORT MODEL)

A 3-D Hybrid analytical – numerical model which includes mass transport, uniform stationary regional flow, 3D dispersion, first order decay, retardation. This model can be used to:

- (i) Predict the concentration in groundwater at a "receptor well",
- (ii) Predict the concentration in groundwater as a source for volatile emissions into a building.

It is appropriate to use this model either when soils data is lacking, or when the groundwater at the source is already impacted and it is not necessary to model the soil-to-groundwater pathway (Spence, 2011 Appendix B).

Assumptions and limitations:

1. The model simulates the transport of dissolved phase contaminants only. It does not simulate the movement of non-aqueous phase liquids (NAPLs).
2. The concentrations estimated by the model represent concentrations in the groundwater aquifer and not concentrations in a pumping well. The concentrations in a pumping well would probably be lower than the concentrations predicted in the aquifer due to dilution effects.
3. The aquifer is considered to be homogeneous and uniform, as well as being infinite in thickness and width.
4. Water table fluctuations are assumed to have no influence on the flow field of the aquifer. The flow direction is uniform and 1-D.

3.2.4.3 Johnson & Ettinger indoor air model

A 1-D analytical exponential model for the migration of vapor from subsurface soil through a cracked foundation, based on a paper by Johnson and Ettinger (1991). It combines a model for both diffusive and advective transport through the soil with a simple model of transport through a building foundation. Advection is caused by a slightly reduced pressure (versus atmospheric pressure) inside a building due to temperature differences, wind, barometric pressure fluctuations or a slight vacuum created by a basement heating system during operation (Spence, 2011 Appendix D).

Assumptions and limitations:

1. A steady-state model with an infinite source (mass is not conserved). This assumption is valid if the source is large compared to the mass flux rate into the building. This assumption has only a minor impact on the risk due to non-carcinogens (unless the source is very small) since the highest seven-year running average intake is compared to the reference dose. It can have a more significant impact however on carcinogens (such as benzene) since the cumulative exposure

over a long exposure duration (up to 30 years) forms the basis for the risk calculation.

2. This model is not linked with any other fate and transport model in RISC.
3. Biodegradation of the chemical vapors is not considered. This is appropriate for chemicals that do not degrade readily, for very short diffusion distances, and/or for screening level calculations.
4. The source is located in the vadose zone. For sources located in the saturated zone the volatilization from groundwater model would be more appropriate.

3.2.4.4 Vapor transport from groundwater into buildings

Similar to the Johnson & Ettinger model described in [section 3.2.4.1](#) above, but with a source located in the groundwater. In this case, the soil gas concentration is calculated from the groundwater concentration by multiplying the groundwater concentration and the chemical's Henry's Law coefficient.

3.2.4.5 Outdoor box model

A 1-D Analytical – Linear model which assumes that the volatile emissions leaving the contaminated soil enter a box shaped area directly overlying the soil. The box is assumed to be ventilated by the wind and the contaminant is fully mixed.

The output of the model is concentration in outdoor air.

Assumptions and limitations:

1. The outdoor air model is for on-site exposures only and does not consider receptors located downwind or distant from the source area.
2. The size of the box should reflect a reasonable exposure area and the exposure duration used should be consistent with the time spent in the box by the potential receptor.
3. The length of the box should never be set to a value less than the respective length of the soil or groundwater source.
4. The air is considered to be fully mixed at all times.
5. The wind speed ventilates the box at a constant rate.
6. The model uses the volatile emission rate calculated by the unsaturated zone model as a source term. This means that the volatile emission rate changes (decreases) every time step as the soil concentration decreases.
7. Does not account for degradation.

3.2.4.6 Particulate emissions model

The particulate emissions (or dust) model is used to predict the concentration of dust particles in the breathing zone directly overlying contaminated surface soil. This pathway is usually only important for non-volatile organic and inorganic contaminants, such as metals.

3.2.5 RBCA Tool Kit

The RBCA Tool Kit consists of a series of linked workbooks designed to operate from within Microsoft Excel, for calculation of baseline risk levels (forward mode) and/or

cleanup levels (backward mode) for soil and groundwater remediation (Connor et al., 2007).

3.2.5.1 Models

The RBCA Tool Kit software package contains a series of fate and transport models for predicting the concentration of chemicals of concern at points of exposure located downwind or down gradient of source areas for air or groundwater exposure pathways, respectively.

Based on representative concentrations of constituents of concern (COCs) present in the affected source media, maximum steady-state concentrations likely to occur at the point of exposure (POE) are calculated using the steady-state analytical fate-and-transport models identified in Appendix X3 of ASTM E 2081-00. To perform these calculations, the system evaluates cross-media partitioning (e.g., volatilization from soil to air) and lateral transport from the source to the POE (e.g., contaminant transport via air or groundwater flow).

In addition to the steady state calculations, an optional Transient Domenico Worksheet² is provided to allow the user to estimate the time required for site constituents to impact off-site groundwater POEs (Connor et al., 2007).

The Johnson & Ettinger model is incorporated also in the RBCA tool kit.

For more details on the transport models see "RBCA Tool Kit for Chemical Releases Version 2" (Connor et al., 2007).

3.2.5.2 Output

Exposure Concentrations: Maximum steady-state concentrations likely to occur at the point of exposure (POE) are calculated using the steady-state analytical fate-and-transport models identified in Appendix X3 of ASTM E 2081-00 (2010).

Average Daily Intake: Based upon the exposure factors selected by the user, the average daily chemical intake for each receptor along each selected pathway is calculated in accordance with USEPA guidelines. These values are used in baseline risk calculations for each complete pathway.

Baseline Risk Characterization: Human health risks associated with exposure to COCs are calculated by the software on the basis of average daily intake rates and the corresponding toxicological parameters for carcinogenic and non-carcinogenic effects. For each complete pathway, the system output provides both individual and additive constituent results for carcinogens and non-carcinogens.

Media Cleanup Values: The RBCA Tool Kit has the ability to i) compare the site data to Tier 1 Risk-Based Screening Levels (RBSLs), computed using the default parameter values as listed in ASTM E 2081-00, or ii) calculate Tier 2 Site-Specific Target Levels (SSTLs) based on user supplied site information. For each source medium (i.e., affected soil and groundwater), the software reports target concentrations for all complete pathways and identifies the applicable (i.e., minimum) value for source remediation.

² For further reading on the Domenico model, see section 2.2.2.3 above

3.2.5.3 Assumptions and limitations

1. For the purposes of simplicity and conservatism, steady-state, constant-source models, providing a lower bound natural attenuation factor (NAF) value - corresponding to maximum chronic exposure conditions - are employed under Tiers 1 and 2.
2. Notwithstanding the above assumption, The RBCA Tool Kit includes a source depletion algorithm which allows for the adjustment of SSTLs to account for changes in source mass over time. For some sites, this decrease in constituent concentration can be modeled as a first order decay. The source depletion algorithm applies user-specified values for source mass and source dimensions. The algorithm also applies user-specified or default values for biodegradation rates for individual constituents to determine a first order decay constant for the decrease in source mass based on the rates of volatilization, dissolution or leaching, and biodegradation. The equilibrium partitioning relationships used in the source decay model are based on the assumption that NAPL is not present in the source area. Use of the source depletion algorithm at sites which contain NAPL will result in non-conservative SSTL values.
3. Further assumptions - applicable for each cross media transfer factor - are described in Connor et al. (2007).

3.2.6 Johnson and Ettinger Model (EPA)

A one-dimensional analytical solution to convective and diffusive vapor transports into indoor spaces. Eight different models are provided in MICROSOFT EXCEL formats. The user can select the appropriate spreadsheet corresponding to the vapor source at the site and determine whether to use the screening level spreadsheet (which allows only one soil type above the capillary fringe) or the more advanced version (which allows up to three layers above the capillary fringe). Both the screening-level models and the advanced models allow the user to calculate a risk based media concentration or incremental risks from an actual starting concentration in soil or in groundwater. Inputs to all models include chemical properties of the contaminant, saturated and unsaturated zone soil properties, and structural properties of the building. Data for any chemical may be edited, new chemicals added, or existing chemicals deleted from the Chemical Properties Lookup Table within the VLOOKUP worksheet. To begin an editing session, the user must unprotect (unseal) the worksheet (the password is "ABC" in capital letters); editing of individual elements or addition and deletion of chemicals may then proceed. The user is also able to adjust parameters relating to building dimension, soil type and depth of contaminant to ensure the fate and transport algorithm reflects the site being assessed.

The Model for soil gas contamination allows the user to input measured soil gas concentration and sampling depth data directly into the spreadsheet. However, this model does not allow for reverse-calculation of a risk-based soil or groundwater concentration.

The Model for Non Aqueous Phase Liquids is designed to forward calculate incremental cancer risks or non-carcinogenic hazard quotients due to subsurface soil vapor intrusion into buildings. The model is specifically designed to handle nonaqueous phase

liquids or solids in soils. The user may specify up to 10 soil contaminants, the concentrations of which form a residual phase mixture. A residual phase mixture occurs when the sorbed phase, aqueous phase, and vapor phase of each chemical have reached saturation in soil. Concentrations above this saturation limit for all of the specified chemicals of a mixture will result in a fourth or residual phase (i.e., nonaqueous phase liquid or solid) (Environmental Quality Inc., 2004).

3.2.6.1 The model

The J&E Model is a one-dimensional analytical solution to convective and diffusive vapor transport into indoor spaces. The model is constructed as both a steady-state solution to vapor transport (infinite or non-diminishing source) and as a quasi-steady-state solution (finite or diminishing source) (Environmental Quality Inc., 2004).

The algorithm uses building properties and soil properties to express the proportionality between the concentration in soil vapour and the consequent concentration in indoor air. It derives two related factors, which are, Q : building, the volume of air exchange moving through the building (expressed as litres per minute) and Q : soil, the volume of vapour moving through the soil into the building (also expressed as litres per minute). The ratio of these two factors leads to the 'soil vapour to indoor air attenuation factor', or alpha (α). This algorithm assumes that there is a ground bearing slab and the groundwater source is directly beneath the building.

3.2.6.2 Output

The RESULTS worksheet shows the indoor exposure soil or groundwater concentration for either a carcinogen or non-carcinogen as appropriate. When a contaminant is both a carcinogen and a non-carcinogen, the risk-based indoor exposure concentration is set equal to the lower of these two values. In addition, the soil saturation concentration (C_{sat}) or the aqueous solubility limit (S) is also displayed for the soil and groundwater models, respectively.

No graphical output is available.

3.2.6.3 Assumptions and limitations

1. The J&E Model does not account for contaminant attenuation (biodegradation, hydrolysis, sorption, and oxidation/reduction), thus EPA is not recommending that the J&E Model be used for sites contaminated with petroleum products if the products were derived from Underground Storage Tanks.
2. Homogeneous soil layers with isotropic properties that characterize the subsurface.
3. All but one of the spreadsheets (the advanced model for a bulk soil source) assumes an infinite source.
4. In the groundwater and bulk soil models, the vapor concentration at the source is calculated assuming equilibrium partitioning.
5. Vapor from the source is assumed to diffuse directly upward (one-dimensional transport) through uncontaminated soil (including an uncontaminated capillary fringe if groundwater is the vapor source) to the base of a building foundation,

where convection carries the vapor through cracks and openings in the foundation into the building.

6. Both diffusive and convective transport processes are assumed to be at steady state.
7. The model should not be used if any of the following conditions exist at the site:
 - a. Presence or suspected presence of Non Aqueous Phase Liquids (NAPLs);
 - b. Heterogeneous geology, fractured media, karst or macropores;
 - c. Sites where significant lateral flow of vapours may occur (e.g., utility conduits);
 - d. Very shallow groundwater that wets building foundation;
 - e. Very shallow groundwater source;
 - f. Very small building air exchange rates (e.g., $<0.25/\text{hr}$);
 - g. Buildings with crawlspaces, earthen floors, stone floors, etc.;
 - h. Contaminated groundwater sites with large fluctuations in water table elevations; and
 - i. Sites with time-varying flow rates and/or concentrations for which a steady state assumption is not conservative.

3.2.7 IRBCA

The Israel Risk-Based Corrective Action (IRBCA) software program is a Microsoft Excel workbook for calculation of baseline risk levels (forward mode) and/or cleanup levels (backward mode) for soil and groundwater remediation, suitable for the Israeli standards.

3.2.7.1 The models

Models included in the IRBCA are as follow:

- Indoor inhalation of vapors from subsurface soil and groundwater – Johnson and Ettinger (J&E) model.
- Outdoor inhalation of vapors from soil – Volatilization factor presented in the Soil Screening Guidance: User's Guide (USEPA, 1996);
- Outdoor inhalation of particulates from soil – Particulate emission factor presented in the Soil Screening Guidance: User's Guide (USEPA, 1996);
- Groundwater protection pathway – Summer model (ASTM, 1995) and Domenico model (Domenico and Swartz, 1990).

3.2.7.2 Output

The output includes tables of calculated risk (forward mode) and target levels (backward mode) for different sort of receptor such as child, resident, non-residential worker etc. and different exposure pathways (inhalation of indoor and outdoor air, dermal contact and domestic use of groundwater etc.).

No graphical output is available.

3.3 Evaluation scenarios

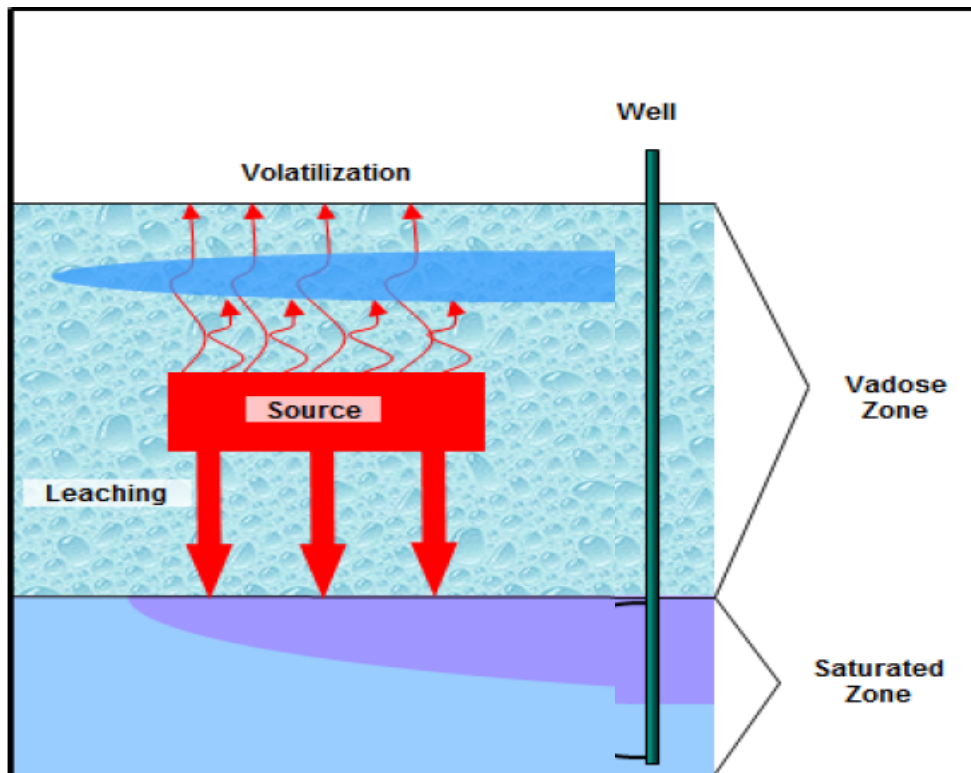
Three scenarios were set in order to compare between the software programs. The scenarios differ by the location of the source of contamination (e.g., vadose zone or groundwater), and as a result by the pathway (the means by which the contamination at the source affects the defined receptor).

1. Scenario 1 – contamination in the vadose zone

A vadose zone of approximately 15 meter thickness was contaminated by TCE (initial concentration of 12.8 mg/kg). The extent of the source is 10 meters by 10 meters with a thickness of 2 meters. The location of the source in the vadose zone ranges from 1 meter below ground surface (b.g.s.) to 10 meters b.g.s. A pumping well and a residential building are situated onsite. The initial condition assumes a non-contaminated saturated zone and vadose zone (beneath and above the source). The following transport pathways were examined (see Figure 3.3):

- Transfer of constituents from soil to groundwater;
- Vapor migration from soil to ambient air;
- Vapor migration from soil to enclosed spaces and indoor air;

Figure 3.3.1: **Examined transport pathways in scenario 1**



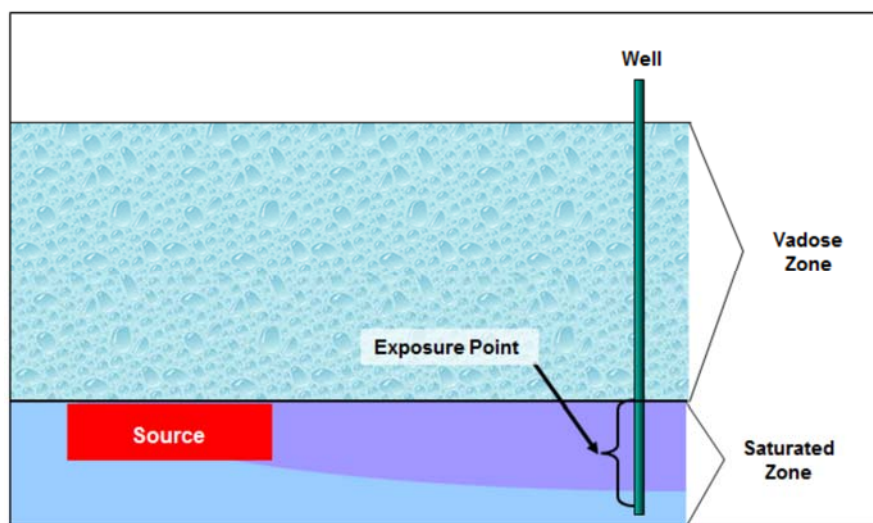
2. Scenario 2 – contamination in the saturated zone, transport in the aquifer

A saturated zone, located about 15 meters below ground surface, was contaminated by TCE (initial concentration of 12.8 mg/L, 1% of the chemical solubility in water). The extent of the source is 10 meters by 10 meters with a thickness (mixing zone) of 2 meters.

The source is assumed to be non-depleting and non-degrading (decay rate = 0). The POEs are two wells, located 150 meters and 1,000 meters down gradient from the contamination source. The vadose zone is assumed to be non-contaminated at the beginning of the simulation.

The transport pathway examined was solute transport down gradient to a well.

Figure 3.3.2: **Examined transport pathways in scenario 2**



3. Scenario 3 – contamination in the saturated zone, migrating to indoor air

Scenario 3 is a continuation of scenario 2 with a transport pathway of vapor migration from groundwater to indoor air - the TCE plume will vapor into the vadose zone and from there into buildings as illustrated in [Figure 3.3.2](#).

Initial concentrations of TCE in groundwater were taken from the results of Scenario 2 from the Tool Kit software.

Figure 3.3.2: **Examined transport pathways in Scenario 3**

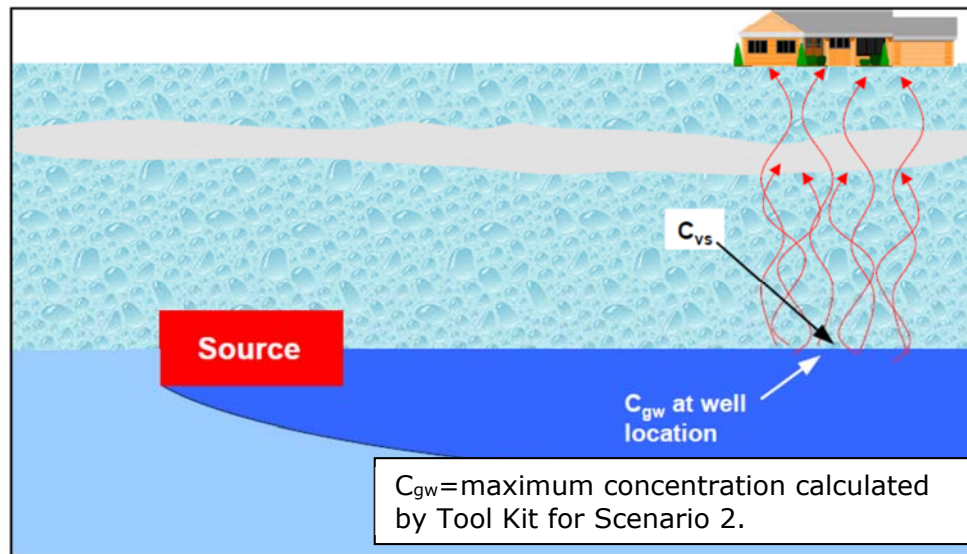


Table 3.3-1 summarizes the scenarios, pathways and programs used.

3.3.1 Data base used for the scenarios

In general, 4 types of data are needed in order to run any of the above programs:

- Exposure parameters and toxicological properties of the constituent;
- Physical and chemical properties of the constituent;
- Physical, chemical and biological properties of the media through which migration occurs;
- Structure of the building through which vapor intrusion occurs;

Values for the above properties were taken from the IRBCA software (see appendix A).

Exceptions from the default values used in the IRBCA were made with the following information:

1. Depth to the saturated zone - 15 meters instead of 3 meters.
2. Source dimension - 10 meters instead of 30 meters.

Table 3.3-1: **Summary of pathways and programs**

Scenario	Source of contamination	Transport pathway	Software program
1	Vadose zone	Transfer of constituents from soil to groundwater; Vapor migration from soil to ambient air; Vapor migration from soil to enclosed spaces and indoor air;	VLEACH, RISC5, RBCA Tool Kit, IRBCA, Johnson & Ettinger (soil model)
2	Saturated zone	Groundwater transport of dissolved constituents	BIOSCREEN, RBCA Tier2 Analyzer, RISC5, RBCA Tool Kit, IRBCA
3		Vapor migration from groundwater to indoor air	Johnson & Ettinger (GW model), RISC5, RBCA Tool Kit, IRBCA

The risk levels used in this work are all based on the default values from the IRBCA software. However, variations in the definitions of the risk levels between the programs result in the need to enter different values in the backward mode as presented in [Table 3.3-2](#).

The variations are as follow:

- In [Tool Kit](#), the individual risk is for each compound and each pathway; therefor it is equivalent to the "IELCR / Hazard Quotient for individual chemical and each exposure pathway" in IRBCA.
- In [RISC5](#), the individual risk is for all pathways of each compound, that is to say if there are multiple exposure pathways, RISC5 will sum the risk contribution from each pathway to get the total risk for an individual chemical; hence, the individual constituent level is corresponding to the "total IELCR / Hazard Index for individual chemical" in IRBCA.
- In [Johnson & Ettinger](#), only one exposure pathway is considered, hence the risk is for each compound and each pathway.

Table 3.3-2: **Target risks definitions**

IRBCA	Tool Kit	RISC5	Johnson & Ettinger	Target Risks used
Potential Carcinogenic Health Effects				
IELCR for individual chemical and each exposure pathway	Individual target cancer risk	---	Incremental risk from vapor intrusion to indoor air	1.0E-06
Total IELCR for individual chemical	---	Individual constituent levels	---	1.0E-05
Total IELCR for each exposure pathway	Cumulative target cancer risk	---	---	1.0E-05
Cumulative site-wide IELCR	---	Cumulative risk	---	1.0E-04
Potential Non-Carcinogenic Health Effects				
Hazard Quotient for individual chemical and each exposure pathway	Individual target hazard quotient	---	Hazard Quotient from vapor intrusion to indoor air	1.0
Hazard Index for individual chemical	---	Individual constituent levels	---	1.0
Hazard Index for each exposure pathway	Cumulative target hazard index	---	---	1.0
Cumulative site-wide hazard index	---	Cumulative risk	---	1.0

4. Results and discussion

Sections 4.1 to 4.3 present the results of the vapor and solute transport models and the risk assessment models (where applicable) from the software platforms examined. Each section deals with a different scenario (soil to groundwater; transport in groundwater and migration from groundwater to ambient and outdoor air).

4.1 Scenario 1 – contamination in the vadose zone

Scenario 1 was run on the following software programs:

- VLEACH
- RISC5
- RBCA Tool Kit
- IRBCA
- Johnson & Ettinger

The VLEACH model³ simulates leaching from the vadose zone to the groundwater but does not include a transport model in the groundwater.

For Scenario 1, the soil model from the Johnson & Ettinger set of Excel files was chosen. The risk values and target levels from this model refer only to the inhalation of indoor air exposure route.

In the RISC5 program, the volatile emission to indoor air exposure pathway was not examined due to limitations of the vadose zone model.

In the IRBCA program, the representative concentrations (RC) for indoor and outdoor inhalation of vapor emissions are the initial concentration of the source in the vadose zone – 12.8 mg/kg.

For the dermal contact and domestic use of groundwater exposure routes, the calculated concentrations in groundwater from the Tool Kit software were used.

The output type differs between the programs. With this restriction, five comparisons can be made:

- A. Maximum mass flux and cumulative mass to groundwater: VLEACH and RISC5 are the only two programs reporting this data (see Graphs 4.1.1.1-4.1.1.2).
- B. Maximum concentration in leachate: comparison between the concentration of the liquid phase in the most lower cell in the VLEACH model and the leachate concentration from the RISC5 model (see Graph 4.1.2).
- C. Maximum concentration in groundwater: results were compared between RISC5 and Tool Kit (see Graph 4.1.3).

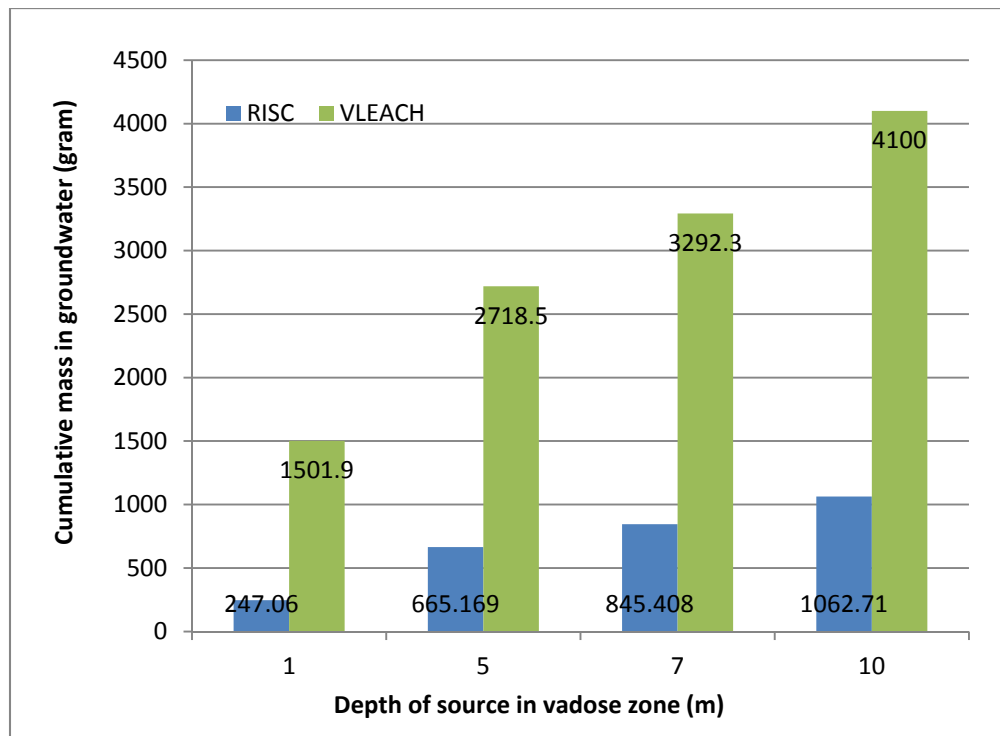
³ Some aspects of the VLEACH model are being re-examined with the software's developers, hence results presented for the VLEACH program should be handled with care.

- D. Comparison of the risk assessment values: implementing the results from Tool Kit in IRBCA and comparing the results from RISC5, Tool Kit, Johnson & Ettinger and IRBCA (see [Graph 4.1.4](#)).
- E. Comparison of the target levels: results from the backward mode calculations to determine the clean-up levels required at the site (see [Graph 4.1.5](#)).

4.1.1 Cumulative mass flux to groundwater

1. The cumulative mass to groundwater in VLEACH is about 3-4 times larger than the cumulative mass in RISC5 (vadose zone model).
2. The closer the source is to the water table, more mass will reach the groundwater.

Graph 4.1.1: **Cumulative mass in groundwater, comparison between VLEACH and RISC5**



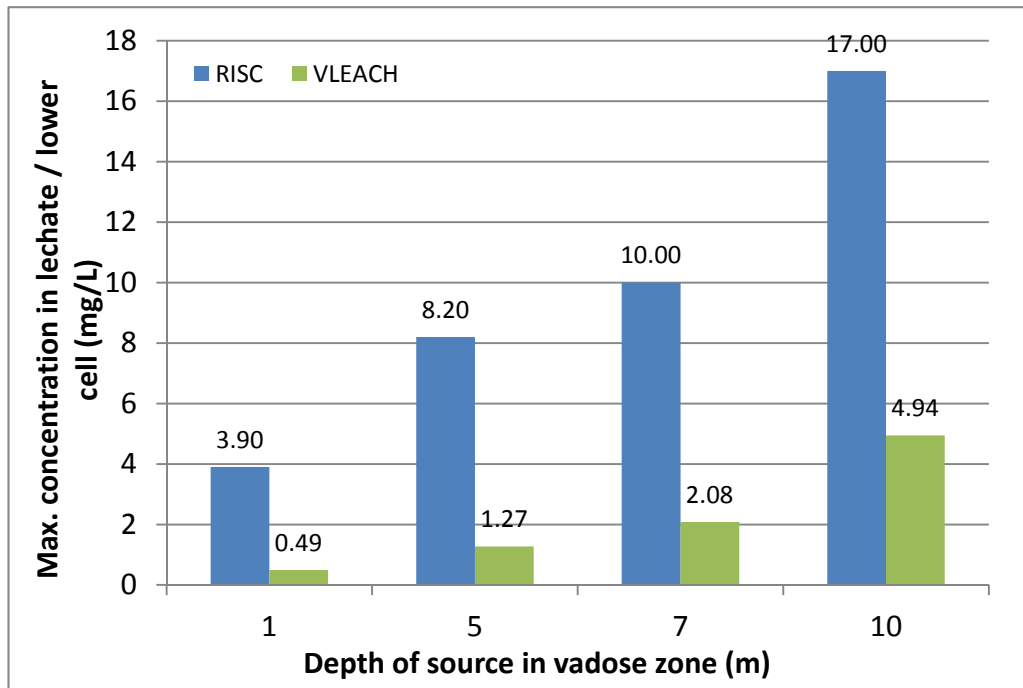
4.1.2 Maximum concentration in leachate

The leachate's concentration in RISC5 and the concentration of the liquid phase in the lowest cell in the VLEACH model were compared.

1. The concentrations increased as the source of the contamination was located closer to the water table.
2. Concentrations were higher in RISC5 than in VLEACH.

3. The time of arrival to maximum concentration (not presented in the graph) ranged between 3-6 years in VLEACH and 4-13 years in RISC5.

Graph 4.1.2: **Maximum concentration in liquid phase, comparison between VLEACH and RISC5**

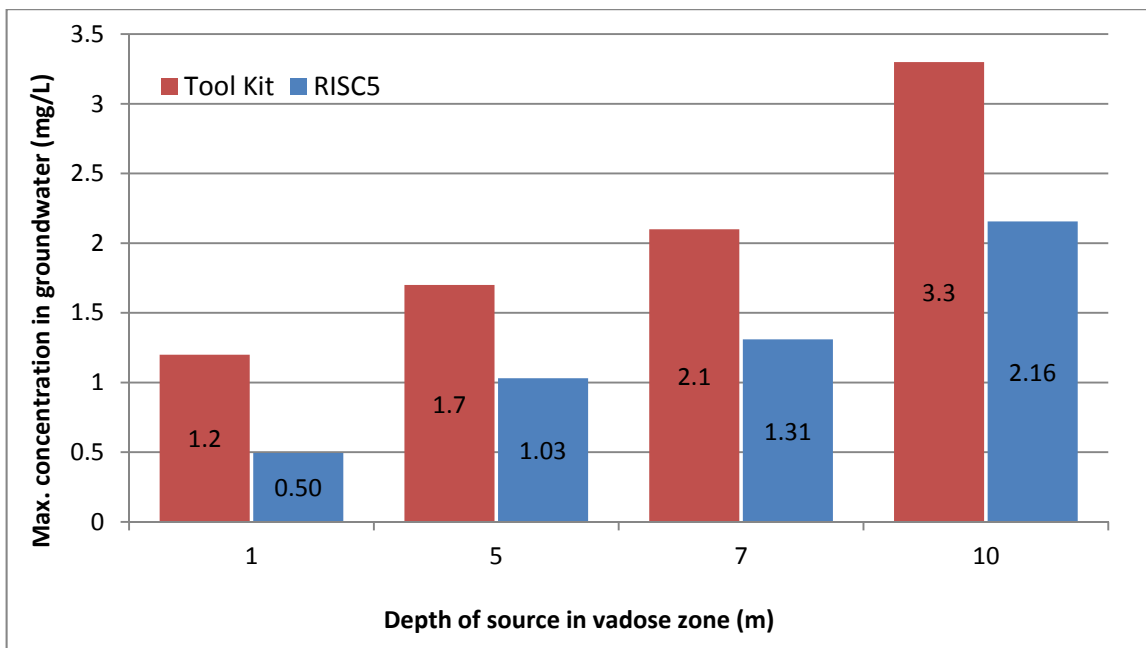


4.1.3 Maximum concentrations in groundwater

Results from Tool Kit and RISC5 were compared:

1. There is a direct relation between the depth of the source and the maximum concentration in groundwater – the deeper the source is (in the vadose zone) the higher the concentrations.
2. In both programs the concentrations were similar, ranging between 0.5 mg/L to 2.2 mg/L in RISC5 and 1.2 mg/L to 3.3 mg/L in Tool Kit.

Graph 4.1.3: **Maximum concentration in groundwater, comparison between Tool Kit and RISC5**



4.1.4 Comparison of risk assessment values (forward mode calculation)

In Tool Kit, the risk levels are displayed separately for each exposure route. This is based on the approach that risks from different routes can't be summed; in RISC5 and IRBCA the risk levels are presented for each exposure route and also as a sum of all risks; risks from the Johnson & Ettinger model are only for inhalation of indoor air. Due to these different approaches in presentation of the risk levels, is divided according to the exposure routes.

1. In Tool Kit, the natural attenuation factor for transport of COCs from the vadose zone to the air (NAF_{cm}) is not reliant upon the initial depth of the contamination, thus for inhalation of indoor and outdoor air, the risk levels do not change with depth.
The NAF between the vadose zone and the saturated zone does change with the initial depth of the contaminant, hence the risk levels for water use increase with depth (see [Graph 4.1.4](#)).
2. In RISC5, the exposure concentration used to calculate the risks for carcinogens is averaged over the total exposure duration (24 years). For non-carcinogens, the exposure concentration is calculated as the worst-case average over 7 years.
In the vadose zone model, a finite mass source is assumed, thus the averaged concentration will be lower than the maximum concentration presented in [Graph 4.1.4](#).

In Tool Kit and IRBCA the source is assumed to be infinite, thus the concentration remains constant with time and is the maximum concentration presents above.

These basic differences are expressed in the risk levels calculated by RISC5 compared to the other two programs (lower risks in RISC5; [Graph 4.1.4](#)).

3. Risk levels for inhalation of outdoor air are similar in RISC5 and Tool Kit.
4. HQ levels for inhalation of indoor air are similar in all three programs (IRBCA, J&E and Tool Kit); cancer risks for this exposure route are much higher in J&E compared to the other programs.
5. Risk levels for dermal contact with water were calculated in two programs – IRBCA and RISC5. Higher exposure concentrations result in higher risks, thus results from IRBCA are higher than those calculated in RISC5.
6. Risk levels for domestic use of water were compared between three programs – Tool Kit, IRBCA and RISC5. As in the dermal contact exposure route, the lowest risks were calculated in RISC5 ([Graph 4.1.4](#)).

Graph 4.1.4: **Carcinogenic risks for ingestion of groundwater**

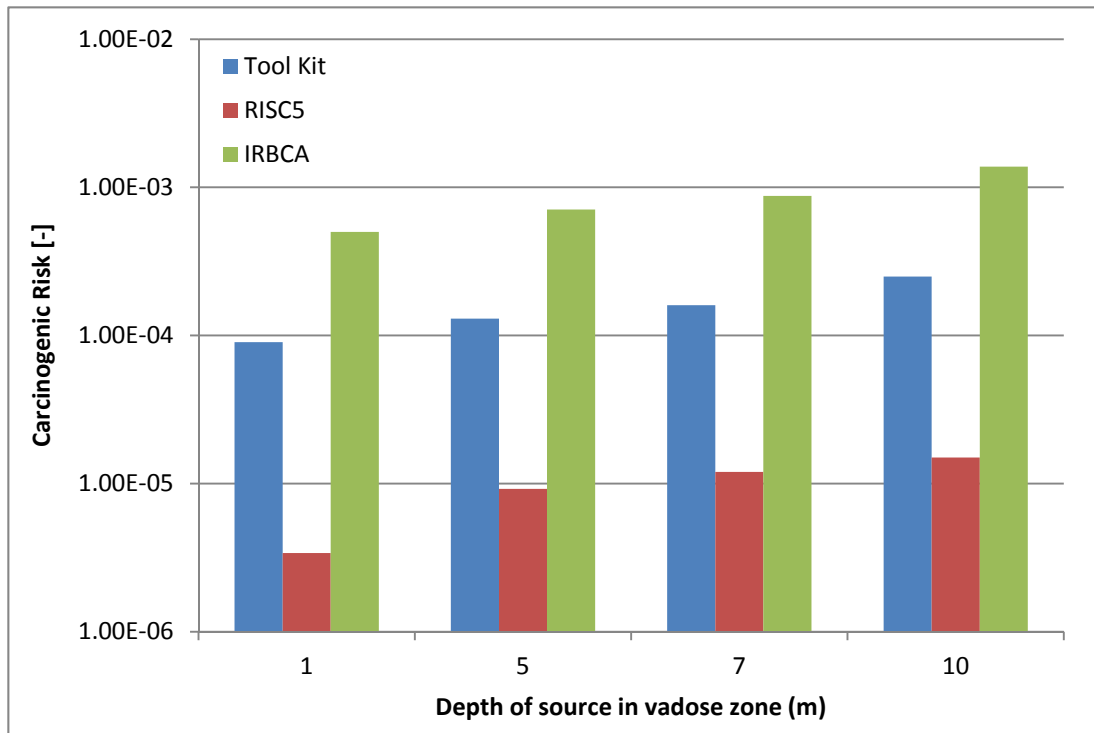


Table 4.1.4: Risk levels by exposure routes

Exposure route: Inhalation of outdoor air

Program	Depth of source in vadose zone (m)							
	10		7		5		1	
	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk
Tool Kit	5.50E-03	3.80E-08	5.50E-03	3.80E-08	5.50E-03	3.80E-08	5.50E-03	3.80E-08
RISC5	3.80E-03	1.60E-08	4.10E-03	1.70E-08	4.30E-03	1.80E-08	4.90E-03	2.00E-08

The IRBCA and J&E programs do not calculate risks for outdoor air inhalation.

Exposure route: Inhalation of outdoor air

Program	Depth of source in vadose zone (m)							
	10		7		5		1	
	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk
Tool Kit	1.60E+01	1.10E-04	1.60E+01	1.10E-04	1.60E+01	1.10E-04	1.60E+01	1.10E-04
IRBCA	5.38E+02	4.61E-03	7.66E+02	6.57E-03	1.07E+03	9.15E-03	5.01E+03	4.29E-02
J&E	9.68E+02	3.65E-01	1.34E+03	5.06E-01	1.80E+03	6.80E-01	5.8E+03	2.2E+00

The vadose zone model in the RUSC5 program does not calculate risks for indoor air inhalation.

Exposure route: Dermal contact with water

Program	Depth of source in vadose zone (m)							
	10		7		5		1	
	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk
IRBCA	NA	2.13E-05	NA	1.36E-05	NA	1.10E-05	NA	7.75E-06
RISC5	2.4E-01	9.30E-07	1.8E-01	7.30E-07	1.5E-01	5.70E-07	5.5E-02	2.10E-07

The J&E program does not calculate risks for dermal contact; The Tool Kit program calculates a combined risk for water use – dermal contact and ingestion of water – as shown on the next table.

Exposure route: Ingestion of groundwater

Program	Depth of source in vadose zone (m)							
	10		7		5		1	
	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk	Hazard quotient	Carcinogenic risk
Tool Kit	1.60E+01	2.50E-04	9.7E+00	1.60E-04	7.8E+00	1.30E-04	5.5E+00	9.00E-05
IRBCA	1.22E+02	1.38E-03	7.77E+01	8.76E-04	6.29E+01	7.09E-04	4.40E+01	5.00E-04
RISC5	3.8E+00	1.50E-05	2.9E+00	1.20E-05	2.3E+00	9.20E-06	8.8E-01	3.40E-06

The J&E program does not calculate risks for ingestion of water; risks presented for the Tool Kit program include both ingestion of groundwater and dermal contact.

4.1.5 Comparison of target levels (backward mode calculation)

In the backward mode, the user specifies either target risks or maximum contaminant levels (MCLs) and the software calculates target levels which are the “allowable” source concentrations. For Scenario 1, the risks were calculated in both methods with a MCL of TCE = 0.03 mg/L, based on the allowable value specified in the IRBCA program.

Table 4.1.5: **Target levels**

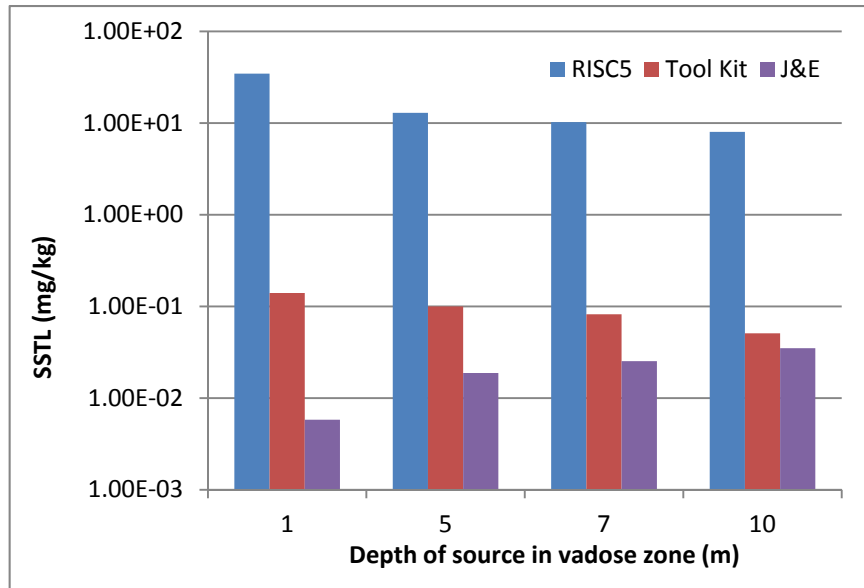
Program	Initial depth of source of contamination (meter)	Target levels based on MCL (mg / kg)	Target levels based on risk levels (mg / kg)
RISC5	1	8.11E-01	3.47E+01
	5	4.08E-01	1.30E+01
	7	3.16E-01	1.02E+01
	10	1.90E-01	8.01E+00
Tool Kit^A	1	3.30E-01	1.40E-01
	5	2.30E-01	1.00E-01
	7	1.90E-01	8.20E-02
	10	1.20E-01	5.10E-02
IRBCA	1	9.32E-02	Program does not calculate target levels based on risks if MCL is given for a constituent
	5		
	7		
	10		
Johnson & Ettinger^A	1	Program does not calculate target levels based on MCLs	5.80E-03
	5		1.88E-02
	7		2.53E-02
	10		3.51E-02

1. The Tool Kit and J&E programs present target levels separately for carcinogenic and non-carcinogenic. In the above table, the minimum levels needed for a site cleanup are presented.

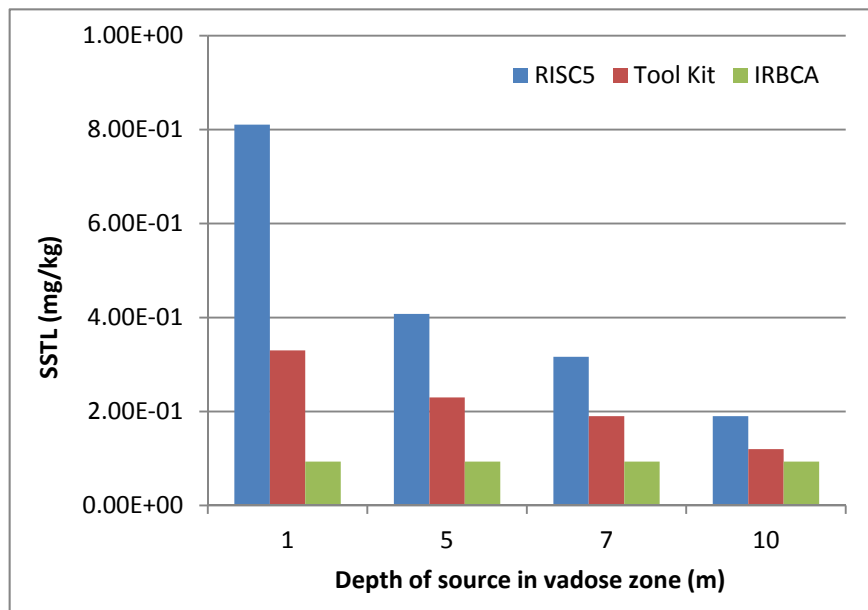
1. The target levels in the RISC5 and Tool Kit programs decreased as the source of the contamination was located closer to the water table. In the J&E program the target levels increased as the source was closer to the water table (see [Graph 4.1.5.1](#)).
2. The target levels based on MCLs calculated in the RISC5 and Tool Kit programs are similar, especially as the source is located closer to the water table. In contrast, target levels based on risks differ greatly, as can be seen in [Table 4.1.5](#).

3. In the IRBCA program, the target levels do not change with depth of the source due to the calculation method used in the program.

Graph 4.1.5.1: **Site Specific target levels (SSTLs) calculated based on risk levels**



Graph 4.1.5.2: **Site Specific target levels (SSTLs) calculated based on MCL**



4.2 Scenario 2 – transport in the saturated zone

Scenario 2 was run on the following programs:

- BIOSCREEN
- RBCA Tier2 Analyzer
- RISC5
- RBCA Tool Kit
- IRBCA

The receptors' locations were set to a distance of 150 meters and 1,000 meters down gradient from the source of contamination.

In the Tool Kit and Tier2 Analyzer programs, the dispersivity changes with the distance from the source and is calculated (automatically by the programs) separately for each receptor using the Xu & Eckstein equation:

$$\alpha_x = 0.83(\log_{10} L)^{2.414}$$

where L is the horizontal length of the plume (10 meters).

For the RISC5 and Bioscreen programs, two runs were made – one for each receptor – and the dispersivity was calculated as a function of the distance to the receptor.

In the IRBCA program the dispersivity is calculated automatically by the software using the ASTM method and cannot be changed by the user. As a result, the dispersivity in this software is higher than that used in the other programs, causing differences in the target levels (see Graph 4.2.3).

In Bioscreen, the soluble mass was defined as infinite.

In IRBCA, the RC used in the forward mode was the maximum concentration in groundwater at the exposure point calculated by the Tool Kit program.

Comparisons of the results are described in sections 4.2.1-4.2.3:

1. Maximum concentration at the exposure point: results were compared between Tier2 Analyzer, Bioscreen, RISC5 and Tool Kit. The point of interest in RISC5 is an actual well (the user enters data on the depth of perforation), while in the other programs, it is an arbitrary point along the centerline of the plume.
2. Comparison of the risk assessment levels: results were compared between the risk assessments models incorporated in RISC5, Tool Kit and IRBCA (Tier2 Analyzer and Bioscreen programs do not include risk assessments tools).
3. Comparison of the target levels: results from the backward mode calculations were compared between Tool Kit and IRBCA.

In addition, Scenario 2 was run also with a lower initial concentration of 1.3 mg/L (0.1% of TCE solubility) and the impact of the initial concentration was examined.

4.2.1 Maximum concentration at a well

1. The RISC5 and Tool Kit programs show similar results of 1.4 mg/L and 1.5 mg/L, respectively for a receptor at a distance of 150 meters and 0.11 mg/L for a receptor at a distance of 1,000 meters.

The Bioscreen program showed somewhat higher concentrations – 3.9 mg/L and 1.05 mg/L for the 150 meters and 1,000 meters receptors, respectively. The tier2 Analyzer program exhibited the highest concentrations (see [Table 4.2.1](#)). These differences are probably the result of different dispersivity values that were entered by the user or calculated by the programs. In future works this issue will be discussed in detail.

The arrival time to peak concentrations ranged between 18 to 30 years and 80 to 130 years for receptors located 150 meters and 1,000 meters, respectively.

Table 4.2.1: **Maximum concentration at the POE**

Model	Max. concentration in POE (mg /L)		Time to reach POE (year)	
	150 m	1000 m	150 m	1000 m
BIOSCREEN	3.9	1.05	30	130
Tier 2 analyzer	8.3	2.8	18	80
RISC5	1.40	0.11	18	90
Tool Kit	1.50	0.11	18	90

1. In RISC5 it is an actual well for which the user enters data regarding the depth of perforation, while in the other programs it is an arbitrary point along the centerline of the plume.

4.2.2 Comparison of the risk assessment values

Carcinogenic risk assessments are similar between all three programs, while the HQ levels calculated by the IRBCA program are higher than those calculated by Tool Kit and RISC5 (see [Table 4.2.2](#)).

Table 4.2.2: **Risk assessments**

Model	HQ		Cancer Risk	
	150 m	1000 m	150 m	1000 m
Tool Kit^A	7.0	0.51	1.1E-04	8.3E-06
RISC5^B	7.1	0.54	8.6E-05	6.6E-06
IRBCA^B	58.5	4.29	6.6E-04	4.8E-05

- A. In the Tool kit program there's no sum of risks and the values listed in the table above represent only risks from groundwater use.
- B. In the IRBCA and RISC5 programs, there's no significant difference between the sum of all risks and the risk from water use. This is due to the small contribution of risks from other exposure routes (e.g., inhalation of indoor and outdoor air).

4.2.3 Comparison of the target levels

The backward mode was run to determine site specific target levels (SSTLs) at the source of contamination, based on maximum concentration levels from the IRBCA software.

1. The Tool Kit program reports SSTLs for each exposure route and for non-carcinogens and carcinogens separately (see [Table 4.2.3-1](#)).
The SSTLs are the allowable concentrations at the source of contamination, depending on the location of the receptors. For example, in order not to exceed a MCL of 0.03 mg/L-TCE in groundwater, the concentration in groundwater at the site should not exceed 0.26 mg/L and 3.5 mg/L for a receptor located 150 meters and 1,000 meters down gradient, respectively.

Table 4.2.3-1: **SSTLs for carcinogens and non-carcinogens, Tool Kit**

Exposure route	receptor distance from source (m)	SSTL for non carcinogens (mg / L)	SSTL for carcinogens (mg / L)
GW ingestion	150	0.26	0.26
	1000	3.5	3.5
Exposure route	receptor distance from source (m)	SSTL for non carcinogens (mg / m3)	SSTL for carcinogens (mg / m3)
Outdoor air inhalation	150	10	1.5
	1000	10	1.5
Exposure route	receptor distance from source (m)	SSTL for non carcinogens (mg / L)	SSTL for carcinogens (mg / L)
GW volatilization to outdoor air inhalation	150	>1.3e+3	>1.3e+3
	1000	>1.3e+3	>1.3e+3
Exposure route	receptor distance from source (m)	SSTL for non carcinogens (mg / m3)	SSTL for carcinogens (mg / m3)
indoor air inhalation	150	11	1.5
	1000	11	1.5

Exposure route	receptor distance from source (m)	SSTL for non carcinogens (mg /L)	SSTL for carcinogens (mg /L)
GW volatilization to indoor air inhalation	150	15	2.2
	1000	200	30

- The IRBCA program reports both the target levels at the receptor location for different exposure routes and the allowable concentration at the source of contamination. The target level for domestic use at the receptor is the MCL for TCE (0.03 mg/L; see [Table 4.2.3-2](#)).

Table 4.2.3-2: **Allowable concentrations at receptor location and at the source of contamination, IRBCA**

Exposure route	Target Levels at receptor (mg /L)	
domestic use	0.03	
Indoor Inhalation of Vapor Emissions	5.83E-02	
Outdoor Inhalation of Vapor Emissions	4.96E+02	
Dermal Contact	1.55E-01	
	SSTL at source of contamination	
Source of contamination	150 meters	1000 meters
Soil Source (mg/kg)	8.55	1.89E+02
Groundwater Source (mg/L)	2.75	1.22E+02

- The RISC5 program reports just the value of the cleanup level needed at the site.

Table 4.2.3-2: **Cleanup levels at the source of contamination, RISC5**

receptor distance from source (m)	Clean-up Levels (mg /L)
150	0.27
1000	3.5

4. The allowable concentrations in groundwater in the IRBCA program are an order of magnitude higher than those calculated in the Tool Kit and RISC5 programs (see Figure 4.2.3).

This difference is due to the different dispersivity values used in the IRBCA program. As can be seen from Eq. 1 (the correlation between allowable concentrations at the POE and target levels), the target levels are greatly affected by the dispersivity values.

Equation 1 -

$$\frac{C(x)}{C_o} = \text{erf} \left[\frac{Y}{4\sqrt{\alpha_y x}} \right] \times \text{erf} \left[\frac{Z}{2\sqrt{\alpha_z x}} \right]$$

$C(x)$ = Dissolved-phase concentration [mg/L]

C_o = Dissolved-phase concentration at the source (at $x=y=z=0$) [mg/L]

α_x = Longitudinal dispersivity [m]

α_y = Lateral dispersivity [m]

α_z = Vertical dispersivity [m]

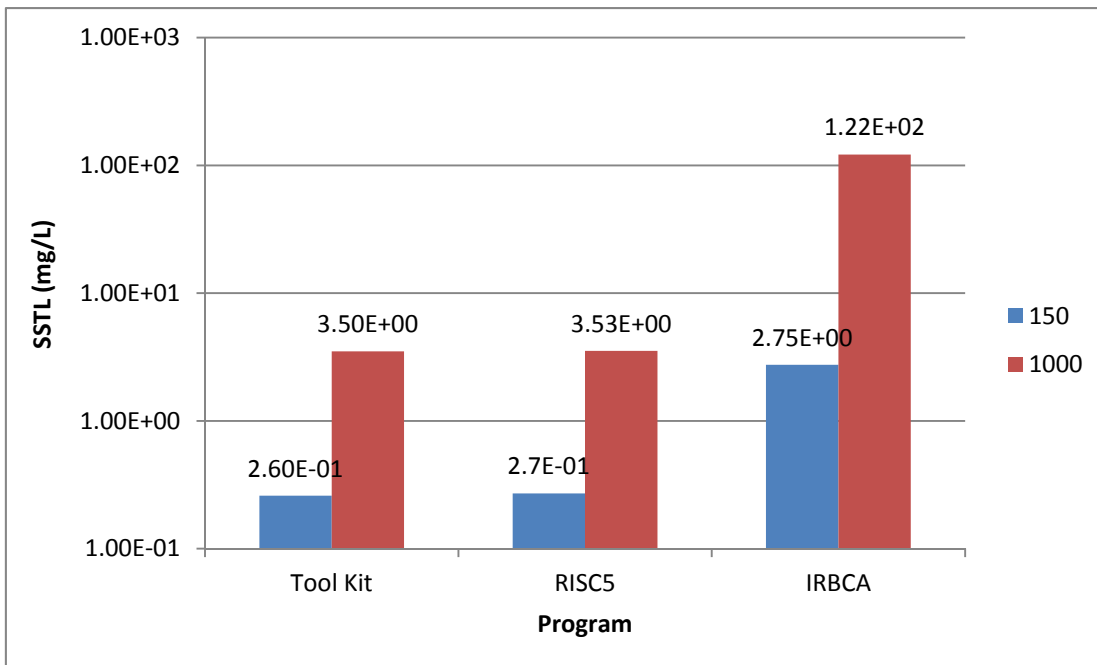
x = Distance along the centerline measured from the downgradient edge of the groundwater source [m]

Y = GW source dimension perpendicular to GW flow direction [m]

Z = GW source (mixing zone) thickness [m]

DA $F_{\text{sat}} = C_o/C(x)$

Graph 4.2.3: **SSTL for groundwater at the source of contamination, comparison between Tool Kit, RISC5 and IRBCA**



4.2.4 The effect of the initial concentration

Under the same assumptions of Scenario 2, a comparison of the programs was made with a different initial concentration – 1.3 mg/L (about 0.1% of TCE solubility).

The decrease of an order of magnitude in the initial concentration resulted in the same change in the maximum concentration and the risk levels. That is, the concentrations are an order of magnitude smaller than those reported in Table 4.2.1 above as do the risk levels.

The target levels remain unchanged because they are not influenced in any way by the initial concentration of the contaminant.

4.3 Scenario 3 – migration of contaminant from the saturated zone to indoor air

Scenario 3 is actually a continuation of the model described in Scenario 2 with the addition of inhalation of indoor air.

The scenario was run on the following programs:

- Johnson & Ettinger (groundwater model)
- RISC5 (forward mode only)
- RBCA Tool Kit
- IRBCA

For RISC5 Tool Kit and IRBCA programs scenarios 2 and 3 were run simultaneously with exposure pathways of dissolved transport in groundwater and volatilization into buildings.

From the three programs examined in this scenario, only the RISC5 has the ability to present concentrations of indoor air, thus this comparison was not carried out.

The initial concentrations in groundwater used in the Johnson & Ettinger program were those calculated by the Tool Kit program in Scenario 2 – 1.45 mg/L and 0.11 mg/L for a receptor located at a distance of 150 meters and 1,000 meters, respectively.

4.3.1 Comparison of risk levels

Results from Scenario 3 include comparisons of the risk and target levels only from the “inhalation to indoor air” exposure route (see Graphs 4.3.1.1 – 4.3.1.2).

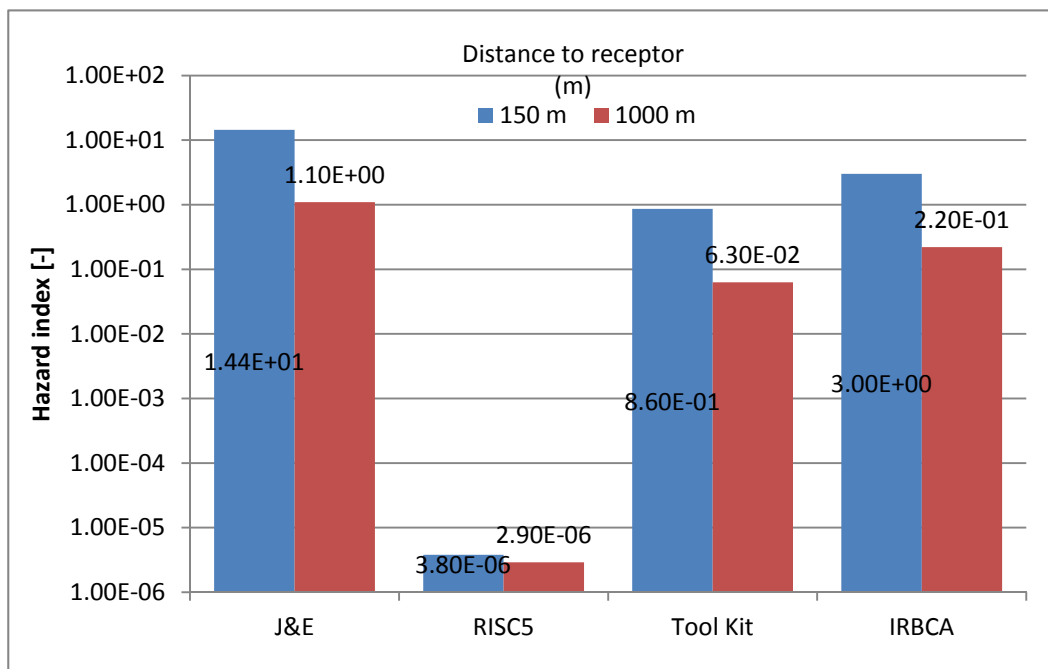
There is great variation in the risk levels between the 4 programs due to the different exposure concentration (the initial concentration of the contaminant in the gaseous phase) used in each program:

Table 4.3.1: **Concentration of TCE in the gaseous phase**

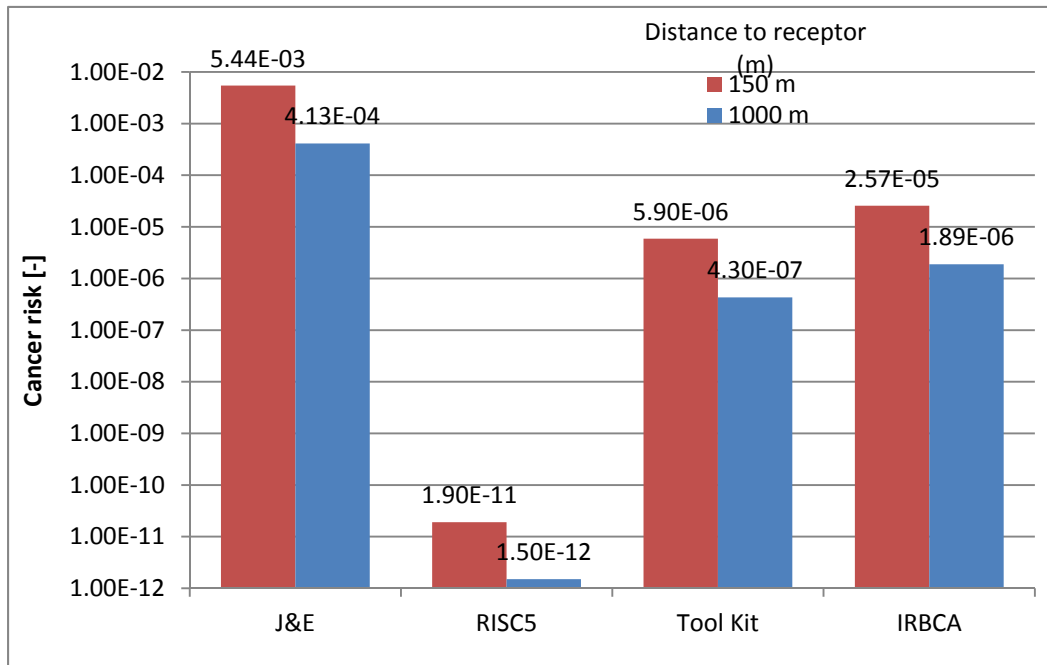
Program	concentration in the gaseous phase (mg / m ³)	
	1,000 meter	150 meter
RISC5	2.9E-09	3.8E-08
Tool Kit	6.4E-04	8.7E-03
J&E	45	593
IRBCA	3.73E-03	5.07E-02

The variations in these concentrations result from different calculation methods embedded in each program.

Graph 4.3.1.1: **Hazard quotient (HQ) levels**



Graph 4.3.1.2: **carcinogenic risk levels**



4.3.2 Target levels

The Johnson & Ettinger program computes only the allowable concentration in groundwater at the receptor location. In the IRBCA program the allowable concentration is set by the program to the Israeli Drinking Water Standard (IDWS) value. In the Tool Kit program both the target levels and the DAF values are calculated so it is possible to calculate also the allowable concentration at the receptor with this ratio - $DAF = C_0/C_x$ and compare with the results from the J&E program (see [Table 4.3.2](#)).

As can be seen in the table, both programs calculated similar allowable concentrations.

Table 4.3.2: **SSTLs, DAF and allowable concentrations**

Program	SSTL (mg / L)		DAF [-]		Allowable concentrations at receptor (mg / L)
	150 m	1000 m	150 m	1000 m	
J&E	---	---	---	---	0.26
Tool Kit	2.2	30	8.6	120	0.25

5. Discussion

The purpose of this deliverable is to evaluate some of the more widely used software platforms in the Risk-Based Corrective Action (RBCA) process.

Seven commonly-used computer software packages were evaluated. The packages are divided in two:

1. Programs which model migration of the constituent: VLEACH, BIOSCREEN, Tier2 Analyzer.
2. Programs which combine both migration models and risk and target levels assessments: RBCA Tool kit, RISC5, Johnson & Ettinger (EPA) and IRBCA⁴.

The software programs were run under three scenarios:

1. Source of contamination located in the vadose zone, leaching towards the groundwater and volatilizing into buildings.
2. Source of contamination in the saturated zone transporting with groundwater to a drinking well.
3. Percolation of contaminant in the gaseous phase from the saturated zone through the vadose zone to buildings.

The programs differ in several aspects – the solution technique (numerical, analytical or a combination of the both); the input data needed by the model of each software; the output types.

A. The solution technique:

The VLEACH program is the only one based on a numerical finite difference model, thus on a mathematical model which requires less assumptions.

All other programs are based on an analytical (or semi analytical) solution of the transport equation, which require many simplifying assumptions to arrive at the solution.

The RISC5 program offers a combination of the analytical and numerical solutions.

B. The input Data:

In general, 4 types of data are needed in order to run the programs:

- o Exposure parameters and toxicological properties of the constituent;
- o Physical and chemical properties of the constituent;
- o Physical, chemical and biological properties of the media through which migration occurs;
- o Structure of the building through which vapor intrusion occurs;

With the first type (exposure parameters) being the hardest to set, as each program ask for somewhat different parameters.

C. The output types:

The three main output types of the programs include:

1. Calculated concentrations at the POE;
2. Risk levels;

⁴ The Johnson & Ettinger and the IRBCA programs have limited capabilities for modeling transport of COC.

3. Target levels for remediation of the site.

The output is given in a table format or a graphical representation or a combination of the two.

1. Calculated concentrations

The concentrations can be given as a function of time or a function of location along the centerline of the plume.

In RISC5 for example, the concentration at the POE is represented as a function of time – $C(t)$ – and the output includes the temporal changes in the concentration of the COC in all the relevant media - the groundwater, the gaseous phase, the leachate and the soil.

In Bioscreen and Tier2 Analyzer on the other hand, the concentration is a function of the location – $C(x)$ – at a specific time point during the simulation time.

2. Risk Levels

The risk levels calculations in all the programs are based on similar equations. However, differences in the concentrations used for these calculations result in variations of the risk levels. The reasons for these differences are shown below:

A. In the IRBCA program the user needs to define the representative concentrations (RC) for each exposure route. With no actual measurements in the field, the RCs used in this work are those resulting from the transport equation in the Tool Kit program or the initial concentrations determined in each scenario.

For example, in Scenario 1, the RC for inhalation of vapors was set to the initial concentration of the scenario (12.8 mg/kg TCE). This concentration is much higher than the ones used in the RISC5 and Tool Kit programs, thus resulting in much higher risk levels (1-2 orders of magnitude) compared to the other two programs.

For exposure routes of dermal contact and ingestion of groundwater, the RCs used in the IRBCA program are those calculated in the Tool Kit program, and the variations in the risk levels are smaller between the programs.

B. The IRBCA and Tool Kit programs use the maximum concentration along the exposure duration, thus resulting in higher risk levels as compared to the risks calculated in the RISC5 program, in which the concentration used is an averaged concentration along the exposure duration.

C. Each program uses different cross-media equations, thus resulting in different concentrations for the same exposure route and of course different risk levels, as was shown in scenario 3.

D. In some programs, the risk levels are the sum of all risks from all exposure routes. Other methodology claims that summation of risks is not possible and one should choose the highest risks from one exposure route.

In the scenarios presented in this work, this difference in methodology (summation of risks or risks by exposure route) was found to be negligible because risks from inhalation of vapors were significantly smaller than those from other exposure routes (mainly domestic use of water).

3. Target levels

The target levels – the concentrations allowable at the site after remediation – can be calculated in one of two ways:

I. Based on target risks;

II. Based on a maximum contaminant level (for example, the Israeli Drinking Water Standard – IDWS).

In this work it was found that when using the MCL to calculate target levels the results are more similar between the programs. This is probably due to the different definitions in which the risk levels are defined in each program.

Even when using the MCL as the base to calculate target levels, the IRBCA program exhibited higher target levels compared to the Tool Kit and RISC5 programs. These differences are the result of the dispersivity values used in the IRBCA program. In this program the dispersivity is calculated by the ASTM method while in the other programs it is calculated using the Xu & Eckstein method or entered manually. The difference in the calculation method resulted in higher target levels in the IRBCA program, compared to the other programs.

Appendix A: Data base used for the scenarios

SITE: 1

BUILDING/ADVECTIVE VAPOR FLUX PARAMETERS FOR VAPOR INTRUSION PATHWAY

Parameter	Symbol	Units	Default	Value Used
Residential Structure				
Surface Area of Building at or Below Grade	A_B	cm^2	Calculated	2.50E+05
Building Ventilation Rate	Q_{bdg}	cm^3/s	Calculated	7.00E+03
Distance from Bottom of Slab to Top of Subsurface Soil	L_T	cm	Calculated	85
Distance from Bottom of Slab to Soil Vapor Measurement			Calculated	85
Distance from Bottom of Slab to Groundwater Table			Calculated	1485
Volumetric Flow Rate of Soil Gas into the Building	Q_{soil}	cm^3/s	83.33	83.33
Q_{soil} is either a user-input above, or calculated below if Q_{soil} above is "NA".				
Volumetric Flow Rate of Soil Gas into the Building	Q_{soil}	cm^3/s	Calculated	
Building Foundation or Slab Thickness	L_{crack}	cm	15	15
Total Area of Cracks	A_{crack}	cm^2	Calculated	200
Soil-Building Pressure Difference	ΔP	$\text{gm}/\text{cm-s}^2$	40	40
Viscosity of Air	μ	$\text{gm}/\text{cm-s}$	Calculated	1.80E-04
Vapor Permeability for Soils below Building	k_v	cm^2	1.00E-08	1.00E-08
Air Exchange Rate	ER	1/24 hr	12.096	12.096
Building Height	H_B	cm	200	200
Building Width	W_B	cm	1000	500
Building Length	L_B	cm	1000	500
Depth below Grade to Bottom of Building Floor	L_F	cm	15	15
Floor-Wall Seam Gap	w	cm	0.1	0.1
Equivalent Crack Radius	r_{crack}	cm	Calculated	0.1
Floor-Wall Seam Perimeter	X_{crack}	cm	Calculated	2000
Non-Residential Structure				
Surface Area of Building at or Below Grade	A_B	cm^2	Calculated	4.00E+06
Building Ventilation Rate	Q_{bdg}	cm^3/s	Calculated	2.76E+05
Distance from Bottom of Slab to Top of Subsurface Soil	L_T	cm	Calculated	85
Distance from Bottom of Slab to Soil Vapor Measurement			Calculated	85
Distance from Bottom of Slab to Groundwater Table			Calculated	1485
Volumetric Flow Rate of Soil Gas into the Building	Q_{soil}	cm^3/s	83.33	83.33
Q_{soil} is either a user-input above, or calculated below if Q_{soil} above is "NA".				
Volumetric Flow Rate of Soil Gas into the Building	Q_{soil}	cm^3/s	Calculated	
Building Foundation or Slab Thickness	L_{crack}	cm	15	15
Total Area of Cracks	A_{crack}	cm^2	Calculated	800
Soil-Building Pressure Difference	ΔP	$\text{gm}/\text{cm-s}^2$	40	40
Viscosity of Air	μ	$\text{gm}/\text{cm-s}$	Calculated	1.80E-04
Vapor Permeability for Soils below Building	k_v	cm^2	1.00E-08	1.00E-08
Air Exchange Rate	ER	1/24 hr	19.872	19.872
Building Height	H_B	cm	300	300
Building Width	W_B	cm	2000	2000
Building Length	L_B	cm	2000	2000
Depth below Grade to Bottom of Building Floor	L_F	cm	15	15
Floor-Wall Seam Gap	w	cm	0.1	0.1
Equivalent Crack Radius	r_{crack}	cm	Calculated	0.1
Floor-Wall Seam Perimeter	X_{crack}	cm	Calculated	8000

The values in red are calculated.

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SITE: 1

EXPOSURE FACTORS

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Parameter	Symbol	Unit	Default Value	Value Used	Comment
Averaging Time for Carcinogen	AT _c	year	70	70	Default Value
Averaging Time for Non-Carcinogen	AT _{nc}	year	=ED	=ED	Default Value
Body Weight:					
Resident Child	BW	kg	15	15	Default Value
Resident Adult	BW	kg	70	70	Default Value
Non-Residential Worker	BW	kg	70	70	Default Value
Construction Worker	BW	kg	70	70	Default Value
Exposure Duration:					
Resident Child	ED	year	6	6	Default Value
Resident Adult	ED	year	24	24	Default Value
Non-Residential Worker	ED	year	25	25	Default Value
Construction Worker	ED	year	1	1	Default Value
Exposure Frequency:					
Resident Child	EF	day/year	360	360	Default Value
Resident Adult	EF	day/year	360	360	Default Value
Non-Residential Worker	EF	day/year	250	250	Default Value
Construction Worker	EF	day/year	90	90	Default Value
Soil Ingestion Rate:					
Resident Child	IR _{soil}	mg/day	200	200	Default Value
Resident Adult	IR _{soil}	mg/day	100	100	Default Value
Non-Residential Worker	IR _{soil}	mg/day	100	100	Default Value
Construction Worker	IR _{soil}	mg/day	100	100	Default Value
Groundwater Ingestion Rate:					
Resident Child	IR _{gw}	L/day	1	1	Default Value
Resident Adult	IR _{gw}	L/day	2	2	Default Value
Non-Residential Worker	IR _{gw}	L/day	2	2	Default Value
Exposure Time for Indoor Inhalation:					
Resident Child	ET _{in}	hr/day	18	18	Default Value
Resident Adult	ET _{in}	hr/day	18	18	Default Value
Non-Residential Worker	ET _{in}	hr/day	18	18	Default Value
Exposure Time for Outdoor Inhalation:					
Resident Child	ET _{out}	hr/day	6	6	Default Value
Resident Adult	ET _{out}	hr/day	6	6	Default Value
Non-Residential Worker	ET _{out}	hr/day	6	6	Default Value
Construction Worker	ET _{out}	hr/day	10	10	Default Value

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SITE: 1

EXPOSURE FACTORS

(Page 2 of 2)

Parameter	Symbol	Unit	Default Value	Value Used	Comment
Skin Surface Area for Dermal Contact with Soil:					
Resident Child	SA	cm ² /day	2800	2800	Default Value
Resident Adult	SA	cm ² /day	5700	5700	Default Value
Non-Residential Worker	SA	cm ² /day	3300	3300	Default Value
Construction Worker	SA	cm ² /day	3300	3300	Default Value
Skin Surface Area for Dermal Contact with Groundwater:					
Resident Child	SA _{gw}	cm ² /day	2800	2800	Default Value
Resident Adult	SA _{gw}	cm ² /day	5700	5700	Default Value
Non-Residential Worker	SA _{gw}	cm ² /day	3300	3300	Default Value
Construction Worker	SA _{gw}	cm ² /day	3300	3300	Default Value
Skin Surface Area for Dermal Whole-Body Contact with Groundwater:					
Resident Child	SA _{wb}	cm ² /day	6600	6600	Default Value
Resident Adult	SA _{wb}	cm ² /day	18000	18000	Default Value
Soil to Skin Adherence Factor:					
Resident Child	M	mg/cm ²	0.2	0.2	Default Value
Resident Adult	M	mg/cm ²	0.07	0.07	Default Value
Non-Residential Worker	M	mg/cm ³	0.2	0.2	Default Value
Construction Worker	M	mg/cm ²	0.3	0.3	Default Value
Event Frequency for Dermal Contact with Soil					
Resident Child	EV _{soil}	event/day	1	1	Default Value
Resident Adult	EV _{soil}	event/day	1	1	Default Value
Non-Residential Worker	EV _{soil}	event/day	1	1	Default Value
Construction Worker	EV _{soil}	event/day	1	1	Default Value
Event Frequency for Dermal Contact with Groundwater					
Resident Child	EV _{gw}	event/day	1	1	Default Value
Resident Adult	EV _{gw}	event/day	1	1	Default Value
Non-Residential Worker	EV _{gw}	event/day	1	1	Default Value
Construction Worker	EV _{gw}	event/day	1	1	Default Value
Event Frequency for Dermal Whole-Body Contact with Groundwater					
Resident Child	EV _{wb}	event/day	1	1	Default Value
Resident Adult	EV _{wb}	event/day	1	1	Default Value
Event Duration for Dermal Contact with Groundwater					
Resident Child	t _{event}	hr/event	1	1	Default Value
Resident Adult	t _{event}	hr/event	1	1	Default Value
Non-Residential Worker	t _{event}	hr/event	1	1	Default Value
Construction Worker	t _{event}	hr/event	1	1	Default Value
Event Duration for Dermal Whole-Body Contact with Groundwater					
Resident Child	t _{wb-event}	hr/event	0.33	0.33	Default Value
Resident Adult	t _{wb-event}	hr/event	0.25	0.25	Default Value

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SITE: 1

FATE AND TRANSPORT PARAMETERS

Parameter	Symbol	Unit	Default Value	Value Used	Comment
SOIL PARAMETERS:					
Soil Source Dimension Parallel to Wind Direction	W_s	cm	1500	1000	Site-Specific Value
Depth to Subsurface Soil Sources from Ground Surface	d_{ss}	cm	100	100	Default Value
Depth of Surficial Soil from Ground Surface	d_s	cm	100	100	Default Value
Depth to Soil Vapor Measurement from Ground Surface	d_{sv}	cm	100	100	Default Value
VADOSE ZONE:					
Total Soil Porosity	θ_t	$\text{cm}^3/\text{cm}^3\text{-soil}$	0.40	0.40	Default Value
Volumetric Water Content	θ_{wv}	cm^3/cm^3	0.10	0.10	Default Value
Volumetric Air Content	θ_{av}	cm^3/cm^3	0.30	0.30	Calculated
Thickness	h_v	cm	29.5	149.5	Calculated
Dry Soil Bulk Density	ρ_s	g/cm^3	1.64	1.64	Default Value
Fractional Organic Carbon Content	f_{ocv}	$\text{g-C}/\text{g-soil}$	0.001	0.001	Default Value
SOIL IN CRACKS:					
Total Soil Porosity	θ_{tcrk}	$\text{cm}^3/\text{cm}^3\text{-soil}$	0.40	0.40	Default Value
Volumetric Water Content	θ_{wcrk}	cm^3/cm^3	0.1	0.1	Default Value
Volumetric Air Content	θ_{acrk}	cm^3/cm^3	0.30	0.30	Calculated
CAPILLARY FRINGE:					
Total Soil Porosity	θ_{tcap}	$\text{cm}^3/\text{cm}^3\text{-soil}$	0.40	0.40	Default Value
Volumetric Water Content	θ_{wcap}	cm^3/cm^3	0.36	0.36	Calculated
Volumetric Air Content	θ_{acap}	cm^3/cm^3	0.04	0.04	Calculated
Thickness	h_c	cm	5	5	Default Value
GROUNDWATER PARAMETERS:					
Depth to GW from Ground Surface	L_{GW}	cm	300	1500	Site-Specific Value
GW Source Dimension Parallel to GW Flow Direction	W_{gw}	cm	3000	1000	Site-Specific Value
GW Source Dimension Perpendicular to GW Flow Direction	Y	cm	3000	1000	Site-Specific Value
Total Porosity in the Saturated Zone	θ_{tss}	cm^3/cm^3	0.4	0.4	Default Value
Dry Soil Bulk Density (Saturated Zone)	ρ_{ss}	g/cm^3	1.64	1.64	Default Value
Fractional Organic Carbon Content in the Saturated Zone	f_{ocss}	$\text{g-C}/\text{g-soil}$	0.001	0.001	Default Value
Groundwater Mixing Zone Thickness	δ_{gw}	cm	153	200	Site-Specific Value
Hydraulic Conductivity in the Saturated Zone	K	cm/year	730000	730000	Default Value
Hydraulic Gradient in the Saturated Zone	i	cm/cm	0.001	0.001	Default Value
Groundwater Darcy Velocity	U_{gw}	cm/year	730	730	Calculated
Infiltration Rate of Water Through Vadose Zone	I	cm/year	21	21	Default Value
AMBIENT AIR PARAMETERS:					
Breathing Zone Height	δ_a	cm	200	200	Default Value
Inverse of Mean Concentration at Center of Square Source	Q/C	$(\text{g}/\text{m}^3\text{-s})/(\text{kg}/\text{m}^3)$	81.64	81.64	Default Value
Fraction of Vegetative Cover	V	m^2/m^2	0.5	0.50	Default Value
Mean Annual Wind Speed	U_{a1}	m/s	3.98	3.98	Default Value
Equivalent Threshold Value of Wind Speed	U_t	m/s	11.32	11.32	Default Value
Windspeed Distribution Function from Cowherd et. al, 1985	$F(x)$	unitless	0.0495	0.0495	Default Value
Volatilization Factor for Domestic Water Use	K_f	L/m^3	0.5	0.5	Default Value

The values in red are calculated.

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SITE: 1

PHYSICAL AND CHEMICAL PROPERTIES OF CHEMICALS OF CONCERN

Chemicals of Concern	Water Solubility	Henry's Law Constant	Org. Carbon Adsorption Coeff.	Soil-Water Sorption Coeff. Vadose Zone	Soil-Water Sorption Coeff. Saturated zone	Molecular Diffusion Coefficient		Saturated Vapor Pressure	Molecular Weight	Saturated Soil Concentration
	(S) [mg/L]	(H) [L·water/L·air]	(K _{oc}) [cm ³ /g]	(K _{ow}) [cm ³ ·water /g·soil]	(K _{ss}) [cm ³ /g]	in air (D ^a) [cm ² /s]	in water (D ^w) [cm ² /s]	(P) [mm Hg]	(MW) [g/g·mol]	[mg/kg]
Trichloroethylene	1.28E+03	4.03E-01	6.07E+01	6.07E-02	6.07E-02	6.87E-02	1.02E-05	7.20E+01	1.31E+02	2.50E+02

NA: Not Available

The values in red are calculated.

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SITE: 1

TOXICOLOGICAL PROPERTIES OF CHEMICALS OF CONCERN

Chemicals of Concern	Oral Slope Factor (SF _o)	Inhalation Unit Risk (IUR)	Dermal Slope Factor (SF _d)	Oral Reference Dose (RfD _o)	Reference Concentration (RfC)	Dermal Reference Dose (RfD _d)	Soil Absorption Factor		Parameters for Dermal Contact Pathway				
							Oral (RAF _o)	Dermal (RAF _d)	Dermal Permeability Constant (Kp)	Relative Contribution of Permeability Coefficient (B)	Lag Time (t _{lagder})	Time to Reach Steady-State (t*)	Fraction Absorbed (FA)
							[-]	[-]	[cm/hr]	[-]	[hr]	[hr]	[-]
Trichloroethylene	5.90E-03	2.00E-06	5.90E-03	NA	1.00E-02	NA	1	NA	1.20E-02	0.051	0.581	1.395	1.000

N/A: Not Applicable
NA: Not Available

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Appendix B: General data on the software platforms

Software platforms	Public Domain / Commercial (price in \$US)	Source / distributor	Tech support (forums, websites, representative etc.)	Known users and projects
VLEACH	Public domain (Free)	Developed by Varadhan Ravi and Jeffrey A. Johnson of Dynamac Corporation. Maintained and distributed by the U.S. EPA, Office of Research and Development, National Risk Management Research Laboratory (NRMRL), Subsurface Protection and Remediation Division (SPRD), Center for Subsurface Modeling Support (CSMoS). www.epa.gov/ada/models.html	Fairly good reply from the Center for Subsurface Modeling Support	1. Nevada Division of Environmental Protection (NDEP) 2. Phoenix-Goodyear Airport federal Superfund site (Arizona) 3. South Africa – An evaluation of GW pollution from pesticides in SA using the VLEACH model
BIOSCREEN	Public domain (Free)	Developed by Groundwater Services, Inc., Houston, Texas, Distributed by Center for Subsurface Modeling Support (CSMoS).	Fairly good reply from the Center for Subsurface Modeling Support	With over 6,000 downloads, it may be the most widely used analytical groundwater model in the world (Cecan et al.) Keesler Air Force Base
RBCA Tier2 Analyzer	Commercial (660\$)	Developed by Doug Cosler, dcosler@coslerconsulting.com (former Waterloo Hydrogeologic, Inc.) Distributor: http://www.groundwatersoftware.com	No web site or forum. Email is available	----

Software platforms	Public Domain / Commercial (price in \$US)	Source / distributor	Tech support (forums, websites, representative etc.)	Known users and projects
RISC5	Commercial (875\$)	Purchasing: 5TU http://www.groundwatersoftware.com/risc5.htm Manufacturer / designer / programmer: Lynn Spence, lynnspace@comcast.net	Fairly good response via email (directly to Lyn Spence, programmer)	As of April 2011, there are over 1,000 users. Amongst them: The US State of Colorado (Oil Inspection Section) RISC5 has been examined by: • UK Environment Agency (2003) • The New Zealand Land care Research Company (2002) • Europe's Network for Industrially Contaminated Land in Europe (NICOLE) • Industrial Sub-Group (Geraghty and Miller, 2004) • Regulatory petroleum site managers at some states of the USA
RBCA Tool Kit	Commercial (895\$)	GSI Environmental Inc.	Tech support available for a price – 75\$ per issue	Luneside Brownfield Regeneration, Lancaster, UK (by AMEC)

Software platforms	Public Domain / Commercial (price in \$US)	Source / distributor	Tech support (forums, websites, representative etc.)	Known users and projects
J&E	PD (Free)	EPA Robert S Kerr Environmental Research Center for Subsurface Modeling Support P.O. Box 1198 Ada, Oklahoma 74821-1198 Phone: (580) 436-8586 Fax: (580) 436-8718 www.epa.gov/ada/models.html	Fairly good reply from the Center for Subsurface Modeling Support	
IRBCA	The software package is not available to public use			