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Remedial Targets Worksheet v3.1: User Manual

Hydrogeological Risk Assessment for Land Contamination.

The Environment Agency is the leading public body protecting and improving the environment in England and Wales.

It's our job to make sure that air, land and water are looked after by everyone in today's society, so that tomorrow's generations inherit a cleaner, healthier world.

Our work includes tackling flooding and pollution incidents, reducing industry's impacts on the environment, cleaning up rivers, coastal waters and contaminated land, and improving wildlife habitats.

This report is the result of research commissioned and funded by the Environment Agency's Science Programme.

Science at the Environment Agency

Science underpins the work of the Environment Agency, by providing an up to date understanding of the world about us, and helping us to develop monitoring tools and techniques to manage our environment as efficiently as possible.

The work of the Science Group is a key ingredient in the partnership between research, policy and operations that enables the Agency to protect and restore our environment.

The Environment Agency's Science Group focuses on five main areas of activity:

- **Setting the agenda**: To identify the strategic science needs of the Agency to inform its advisory and regulatory roles.
- **Sponsoring science**: To fund people and projects in response to the needs identified by the agenda setting.
- **Managing science**: To ensure that each project we fund is fit for purpose and that it is executed according to international scientific standards.
- **Carrying out science**: To undertake the research itself, by those best placed to do it - either by in-house Agency scientists, or by contracting it out to universities, research institutes or consultancies.
- **Providing advice**: To ensure that the knowledge, tools and techniques generated by the science programme are taken up by relevant decision-makers, policy makers and operational staff.

Steve Killeen   Head of Science

Executive Summary

This document has been prepared to support risk assessors using the Remedial Targets Worksheet v3.1, which was developed to accompany the document *'Remedial Targets Methodology: Hydrogeological risk assessment for land contamination'.* The methodology and the MS Excel97^{TM} worksheet, for which this user manual has been prepared, provide a framework for assessing the risks to controlled waters from land contamination, and for deriving remedial targets where those risks are unacceptable. The remedial targets produced by this method should be combined with provisional remedial objectives for all other relevant receptors present at a site, such as humans, flora, fauna and building materials, in order to address all of the risks that may be present on a site as a whole.

The worksheet described has been prepared in MS Excel97^{TM} and no claim is made to its application in Excel2000 or other versions of MS Excel. However, attempts have been made to ensure that the equations included will allow error functions to be correctly calculated in Excel2000.

Contents

1 Introduction

This User Manual has been prepared to assist users of the Environment Agency's Remedial Targets Worksheet v3.1. The worksheet, produced in Microsoft Excel97™, was produced to help risk assessors following the framework set out in the Environment Agency publication *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination* (Environment Agency, 2006a). This worksheet provides an update to earlier versions which were developed to support the framework set out in the document *Methodology for the derivation of remedial targets for soil and groundwater to protect water resources* (Agency, 1999a).

This document describes the functionality of the worksheet and gives guidance on its use. It is not intended to describe the technical basis underpinning environmental risk assessment, the regulatory and policy context within which risk assessments are undertaken, or the Environment Agency's approach to assessing risk assessment reports. The worksheet should only be used by suitably experienced risk assessors who have previously read the *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination,* and who are conversant with the relevant UK legislation, policy and guidance.

2 Obtaining and installing the worksheet

The Remedial Targets Worksheet v3.1 can be downloaded from the Environment Agency's website (www.environment-agency.gov.uk/publications) free of charge.

The worksheet has been prepared and tested in Microsoft Excel97™ on the MS 95/2000/XP operating systems. The file comprises about 810KB, and should not require any significant additional computing capability beyond that needed to run Microsoft Excel97™.

It is recommended that a blank copy of the worksheet (as downloaded from the Agency's website) is saved to a safe file and that each simulation is saved as a distinct file.

In order to enable the worksheet, a number of capabilities are required in Excel that may not automatically be set. The worksheet calculates error functions and complimentary error functions. Before using the worksheet, it may be necessary to add these capabilities by clicking the following from the pull-down Tools menu:

Tools ➜ Add-Ins ➜ Analysis ToolPak *and* Analysis ToolPak-VBA

When the worksheet is first opened, the initial screen will prompt the user to save the simulation in a discrete file location.

3 Overview

The Remedial Targets Worksheet calculates solutions to equations presented in the *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination* (Environment Agency, 2006a). It should only be used in conjunction with that document.

Version 3.1 of the Remedial Targets Worksheet incorporates a number of changes from Version 2, which are summarised below:

- Air- and water-filled porosities can be calculated from moisture content and density data;
- The calculation of the partition coefficients for polar organic compounds has been corrected to include fraction of organic carbon;
- Dilution by groundwater flow only is considered. Dilution in the receptor should be dealt with as described in *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination.*

The scientific basis of these updates is described in detail in the *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination* (Environment Agency, 2006a).

The remedial targets methodology has been developed to help assessors derive site-specific remedial targets for contaminated soils and groundwater that are protective of the wider water environment. The framework does not consider the risks posed by contaminants to other receptors, such as humans (for soil sources), buildings, flora and fauna. However, the risks to these (and any other relevant) receptors need to be considered when developing remedial objectives for a site as a whole. Readers who are unfamiliar with the concepts of environmental risk assessment and the Agency's approach to protection of groundwater are directed to the following documents:
- DETR *et al*, 2000. *Guidelines for environmental risk assessment and management.* The Stationery Office.
- Defra and Environment Agency, 2004. *Contaminated Land Research Report, CLR11: Model procedures for the management of land contamination.*
- Environment Agency, 2006a. *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination.*
- Environment Agency, 2006b. *Groundwater Protection: Policy and Practice (1-3) (consultation version).*

The remedial target methodology and the worksheet have been developed to help assessors derive site-specific remedial targets for sites where soil and/or groundwater are already contaminated as a consequence of past activities and practices. The worksheet should only be used in this context – in particular, due to the requirements of the EU Groundwater Directive and Dangerous Substances Directive it may be inappropriate to use parts of this framework to assess the acceptability of discharges from new or current activities.

Before selecting this, or indeed any other assessment model or tool, assessors should have developed a conceptual model of the site. They should be satisfied that the tool they select to model the site is appropriate, both in respect of representing the

conceptual model and in performing analyses to a level that is appropriate to the quality of the input data. Guidance on these issues is provided in:

- Environment Agency, 2001a. *Guide to good practice for the development of conceptual models and the selection and application of mathematical models of contaminant transport processes in the subsurface.* National Groundwater and Contaminated Land Centre report NC/99/38/2, Solihull.

- Environment Agency, 2001b. *Benchmarking and guidance on the comparison of selected groundwater risk-assessment models.* National Groundwater and Contaminated Land Centre report NC/00/14, Solihull.

The development of a robust conceptual model is perhaps the most important aspect in the process of successfully estimating and evaluating environmental risks. The use of any mathematical modelling tool without first developing a robust conceptual model is likely to result in meaningless output and poor decision-making. **This worksheet should only be employed where a robust conceptual model has been developed, and the assessor is satisfied that the calculations performed by the worksheet are relevant to the processes described within that conceptual model**.

Data quality is also a particular concern. Data used should be relevant, reliable and derived from tests at the site, or be relevant to the site. The provenance and relevance of all data included in an assessment using the worksheet should be documented by the assessor and included in the report(s) submitted to the Agency for consideration. The Agency has produced guidance for its staff on reviewing submitted assessments, and this may be of use to assessors preparing reports for submission to the Agency:

- Environment Agency, 2001d. *Guidance on the assessment and interrogation of subsurface analytical contaminant fate and transport models.* National Groundwater and Contaminated Land Centre report NC/99/38/1, Solihull.

The structure of the assessment framework is described in detail in the *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination,* and is not reproduced here. It is important to remember, however, that as assessors progress through the levels, the point at which compliance is tested will change (Figure 3.1), and the amount of data which must be collected from the site will increase. This worksheet should only be used to derive remedial targets at a level for which adequate site-specific data have been obtained. Note the term level now replaces tier, which was used in the original remedial target methodology, (Agency, 1999).
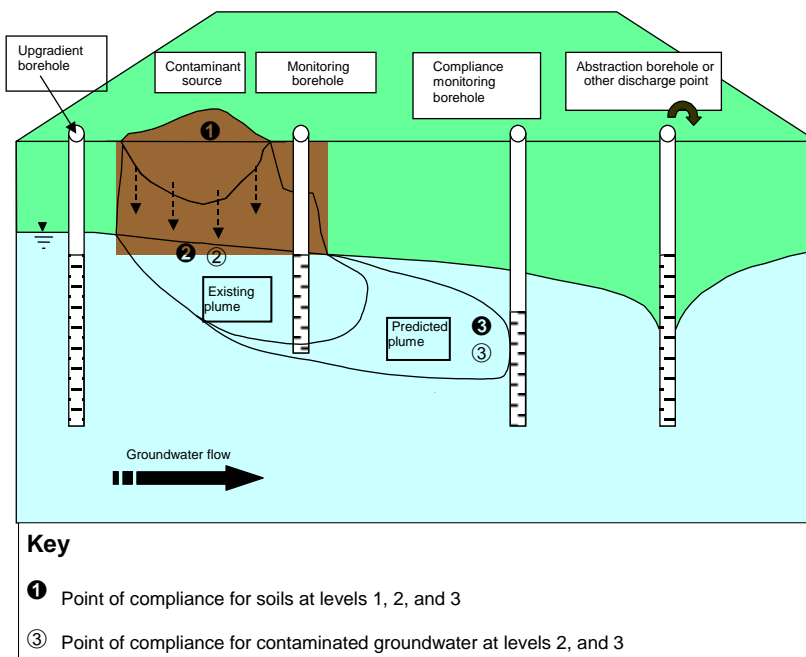
Figure 3.1 Assessment levels and compliance points

This spreadsheet does not include for attenuation in the unsaturated zone or for dilution in a specific receptor such as a receiving watercourse or abstraction borehole. If these elements need to be included in the assessment then this will need to be undertaken using a separate numerical model.

4 Using the worksheet

4.1 General

The Remedial Targets Worksheet v3.1 incorporates 16 sheets, which have the following functions:

Table 4.1 Function of worksheets

Title of worksheet	Function of sheet
Introduction	Brief instructions, entry of site details, assessor details, enter contaminant and water target concentration for transfer to subsequent sheets
Level 1 Soil	Data entry for calculating Level 1 remedial targets for soil, and presentation of results
Level 2 Soil	Data entry for calculating Level 2 remedial targets for soil, and presentation of results
Level 3 Soil	Data entry for calculating Level 3 remedial targets for soil, and presentation of results
Soil impact results	Tabulates predictions of impact on water quality from contaminated soil at each Level
Simple calculations	Data entry and computation of simple hydrogeological calculations
Porosity Calculator	Data entry and calculation of air and water filled porosities
Level 1 Calc	Calculation of Level 1 remedial targets for soil from data input to 'Level 1 Soil'
Level 2 Calc	Calculation of Level 2 remedial targets for soil from data input to 'Level 2 Soil'
Level 3.1 Soil Calc	Calculation of Level 3 remedial targets for soil using the Ogata Banks solution from data input to 'Level 3 Soil'
Level 3.2 Soil Calc	Calculation of Level 3 remedial targets for soil using the steady-state Domenico solution from data input to 'Level 3 Soil'
Level 3.3 Soil Calc	Calculation of Level 3 remedial targets for soil using the time-variant Domenico solution from data input to 'Level 3 Soil'
Level 3 Groundwater	Data entry for calculating Level 3 remedial targets for groundwater, and presentation of results
Level 3.1 G Calc (2)	Calculation of Level 3 remedial targets for groundwater using the Ogata Banks solution from data input to 'Level 3 Soil'
Level 3.2 G Calc (2)	Calculation of Level 3 remedial targets for groundwater using the steady-state Domenico solution from data input to 'Level 3 Soil'
Level 3.3 G Calc (2)	Calculation of Level 3 remedial targets for groundwater using the time-variant Domenico solution from data input to 'Level 3 Soil'

Data entry is only possible in the seven shaded worksheets, and results of each calculation are presented on the relevant worksheet. The remaining worksheets perform the calculations specified within the previous worksheets and are provided so that assessors can follow the mathematical calculations more easily. It is neither possible, nor necessary to modify or enter data into any of the calculation sheets. In principle it is not necessary to open any of the calculation sheets to successfully use this worksheet.

Each worksheet is password protected and data may only be entered in specific cells, which are colour-coded blue, brown or yellow.

Blue cells require data to be entered, to either perform a specified calculation, or to record site details. Data may take the form of either site details as text (on the 'Introduction' sheet) or values for identified parameters on all other sheets. All blue cells must be completed for each assessment type.

Brown cells are pull-down menus where options can be selected to allow the assessor to select a predefined option.

The origin or source of any data used in the worksheet should be recorded in the yellow cells. Although failure to populate the 'Source of parameter value' cells with appropriate text will not prevent calculation of the remedial targets, it is good practice to complete this task. The Environment Agency will expect submitted reports to include these details.

Grey cells contain the results of each simulation and green cells contain information derived from another part of the spreadsheet, which although not essential for the simulation is useful to the assessor.

If the assessor moves the cursor over the red triangles at the corner of certain cells, further information is revealed on the data required or equations solved.

4.2 Introduction worksheet

When starting a new assessment, users **MUST** complete details on the 'Introduction' worksheet first (Figure 4.1). This worksheet is displayed for all assessment options. Data required (in blue boxes) on the 'Introduction' worksheet include:

- Name and address of the site being assessed
- Name of assessor, date that assessment was completed, and run version number
- Name of contaminant
- Target concentration
- Basis for target concentrations (e.g. EQS, DWS, limit of detection).

All blue cells on the 'Introduction' sheet must be completed before moving onto any other worksheets. Data entered for the pollutant name, target concentration, site name, assessor's name, date of assessment and identifying run number are automatically transferred to each of the subsequent data entry sheets. These details can not be amended within the subsequent sheets, and can only be modified by changing the entry on the 'Introduction' sheet.

The 'Introduction' sheet also includes brief instructions on the use of the worksheet and a reminder that Microsoft Excel97™ Tools must be enabled to allow it to calculate error functions and complimentary error functions. The worksheet will not calculate Level 3 remedial targets for soil or groundwater, unless MS Excel™ is set-up to calculate these mathematical functions.

It is necessary to undertake a separate simulation for each pollutant present on a site and for each assessment type (soil, groundwater). Only one substance and assessment should be considered in a single simulation.

Guidance on selecting appropriate target concentrations, which are typically based on background water quality, drinking water standards (DWS) or environmental quality standards (EQS) can be found in '*Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination'*.

Figure 4.1 Data entry required on Remedial Targets Introduction Worksheet

4.3 Level 1 Soil worksheet

The 'Level 1 Soil' worksheet (Figure 4.2) allows assessors to determine Level 1 remedial targets for contaminated soil.

Project information data (site and contaminant details) are automatically transferred to the Level 1 worksheet from the 'Introduction' sheet. Calculation of remedial targets cannot be performed unless the target concentration has previously been entered on the 'Introduction' sheet.

Brown cells: Assessors must first select which approach to the calculation of partition coefficients between soil matter and pore waters is appropriate. Assessors have three options and must select from the pull-down menu located on the brown coloured cell. The three options are:

1. Enter value for partition coefficient (Kd)
2. Calculate Kd for non-polar organic chemicals based on:

$$K_d = K_{oc}.f_{oc}$$

3. Calculate Kd for polar (ionic) organic chemicals based on:

$$K_d = \left\{ K_{oc,n}\left(1+10^{pH-pKa}\right)^{-1} + K_{oc,i}\left(1-\left(1+10^{pH-pKa}\right)^{-1}\right)\right\} f_{OC}$$

The Level 1 remedial target for soil is subsequently calculated as:

$$C_{soil} = C_T\left(K_d + \frac{\theta w + \theta a H}{\rho}\right)$$

The screenshot contains the following callout boxes:

- Select approach to model partition coefficients from the pull-down menu.
- The source of each value should be documented on the worksheet and in associated reports.
- Project data input on the 'Introduction' worksheet are automatically transferred onto subsequent worksheets.
- Level 1 remedial target for soil (as mg/kg in soil) presented.
- Complete each of the blue cells - the cells coloured blue will vary depending on which approach to modelling partitioning of the pollutant has been selected. Other cells are blacked out.
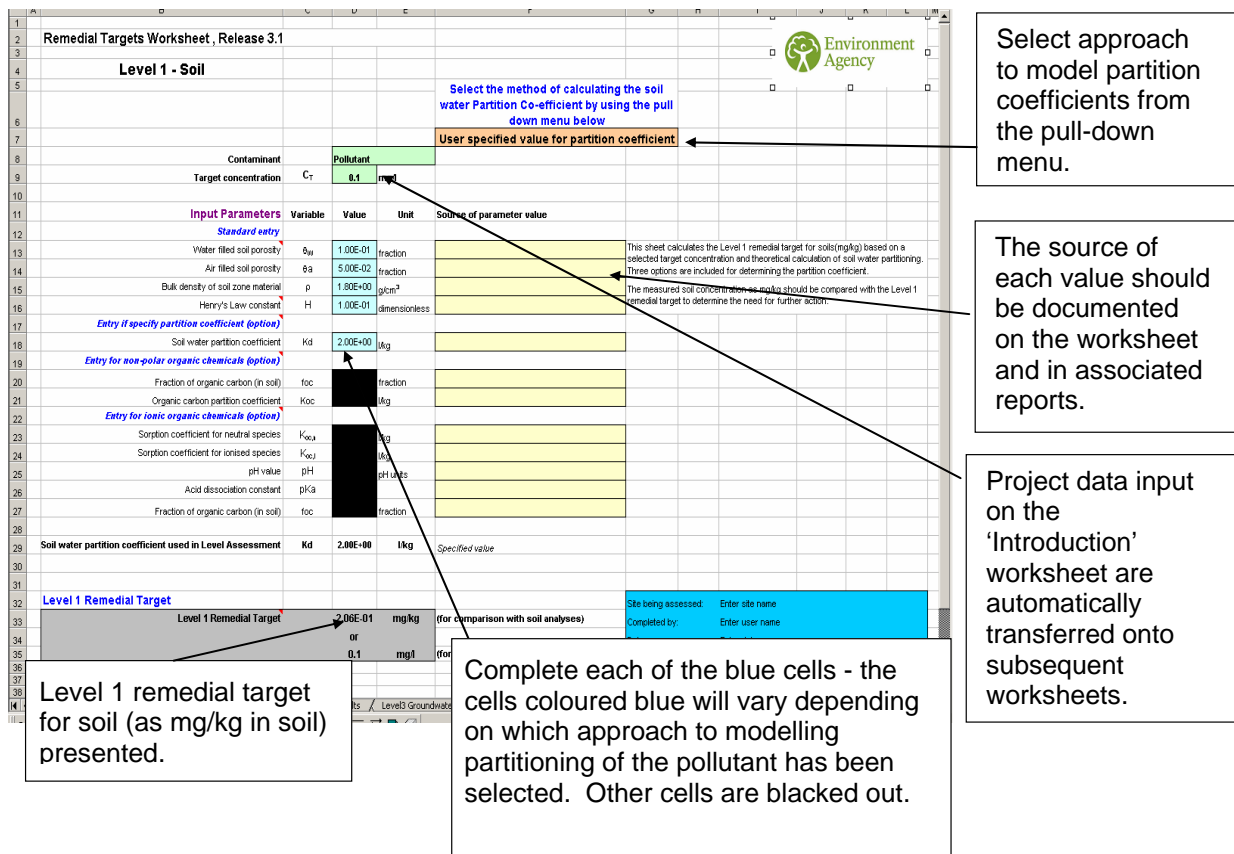
Figure 4.2 Level 1 (Soil) worksheet

Blue cells: Data entry requirements (i.e. blue cells) are determined by the selected approach to modelling contaminant partitioning, as described above. It is only necessary to enter data in the blue cells. Cells where data are not required will be blacked out.

Whichever partition coefficient option is selected, it is still necessary to enter the following data:

1. Water filled soil porosity, θ_w
2. Air filled soil porosity, θ_a
3. Dry bulk density of soil, ρ_{soil}
4. Henry's Law Coefficient (for non-volatile contaminants this should be zero).

It is important to remember that data entered on the Level 1 worksheet relate to materials in the 'source zone', that is to say the porosity, density, fraction of organic carbon etc. values relate to the materials in which contaminants are located. This will normally be soil, made ground or unsaturated rock. If a value for K_d is derived from literature sources, it is important to ensure that it is relevant to the matrix in which contaminants are located at the site being considered. The following list identifies important issues related to each parameter required.

Water filled soil porosity, (θ_w): fraction of the pore space within the source zone material that is filled with water. Expressed as a fraction between 0 and the total porosity value. The water filled porosity value can be derived from water or moisture

content measurement and density measurements. To determine the appropriate water filled porosity complete the 'Porosity Calculator' worksheet, which is described in Section 4.7. This value should then be entered into the appropriate blue cell in the Level 1 worksheet.

Air filled soil porosity, (θ_a): fraction of the pore space within the source zone material that is filled with air. Expressed as a fraction between 0 and total porosity value. Air-filled plus water-filled porosities equal the total porosity of the matrix material. The air filled porosity value can be derived from water or moisture content measurement and density measurements. To determine the appropriate air filled porosity complete the 'Porosity Calculator' worksheet, which is described in Section 4.7. This value should then be entered into the appropriate blue cell in the Level 1 worksheet.

Dry Bulk density,(ρ_{soil}): of the soil /made ground /material in which the contaminant source is located.

Henry's Law Constant: Contaminant specific value that describes the partitioning of a compound between an aqueous solution and the gaseous phase.

Henry's Law Constant should be expressed in the dimensionless form, which can be calculated by multiplying Henry's Law Constant expressed in atm m^3 mol^{-1} by 42.9 (unit conversion at 11°C).

For inorganic chemicals and non-volatile compounds it should be set to zero.

Soil water partition coefficient,(K_d): Contaminant specific value, K_d, that describes the partitioning of a substance between the soil /made ground matrix and surrounding water. Soil water partition coefficients will typically be derived from laboratory column experiments, or field data where comparison with a conservative tracer is possible. If a contaminant is conservative (i.e. it does not sorb to soil or aquifer materials), such as chloride, its K_d value is zero.

Fraction of organic carbon, (f_{oc}): value (as a fraction between 0 and 1) for the soil, made ground or other material in which the contaminant source is located. For example, if there is 0.5% organic matter in an aquifer material, f_{oc} would be 0.005.

Organic carbon partition coefficient, (K_{oc}): Contaminant specific value, K_{oc}, which describes the partitioning of a substance between organic matter and water. An appropriate value must be inserted into the blue cell, if calculating K_d for non-polar ionic compounds.

A conservative organic compound has a K_{oc} value of zero.

Sorption coefficient for neutral species, (Koc,n): onto soil / made ground / matrix in which a contaminant source with polar properties is located.

Sorption coefficient for ionised species, (Koc,I): onto soil / made ground / matrix in which contaminant source with polar properties is located. Positively charged ions generally have a greater potential to sorb to the soil matrix because most subsurface solids have a negative net surface charge.

pH value: of the pore water. Measure of the concentration of hydrogen ions, H^+. Specifically, the negative logarithm of the hydrogen ion concentration.

Acid dissociation constant, (pKa): of an ionised substance in the pore water.

Once data have been entered in all of the blue cells, click away on another cell and the Level 1 remedial target will presented (as mg/kg) in the grey box at the bottom of the screen.

Yellow cells: the origin or source of all data used should be documented. Yellow cells are provided on the worksheet for brief notes of data provenance.

4.4 Level 2 Soil worksheet

The Level 2 Soil worksheet (Figure 4.3) takes data already entered at Level 1 and calculates a Level 2 remedial target that includes a factor for dilution of the contaminants.

Figure 4.3 Level 2 Soil worksheet

The level 2 worksheet allows dilution by groundwater flow below the site to be taken into account in determining the remedial target for contaminated soil (Note: attenuation in the unsaturated zone is not considered in this spreadsheet and should be derived separately).

The equations solved for a dilution factor, DF, at Level 2 are as follows (for explanation of terms in equations see *Remedial Target Methodology*):

$$DF_{GW} = \frac{(K.i.M_z + L.Inf)C_T - (K.i.M_z.C_u)}{L.Inf.C_T}$$

The assessor will also need to select how to determine the thickness of the mixing zone within the aquifer. Two options are given:

1. The thickness of the mixing zone can be calculated using the following solution after USEPA, 1996; or
2. The thickness of the mixing zone can be specified by the assessor.

The empirical calculation for mixing zone thickness is the following relationship:

$$M_z = \sqrt{0.0112L^2} + da\left[1 - \exp\left(\frac{-L.Inf}{K.i.da}\right)\right]$$

The thickness of the mixing zone cannot exceed the saturated thickness of the aquifer. If a value greater than the saturated aquifer thickness is entered, the worksheet posts a warning that "*mixing zone exceeds saturated thickness*".

Generally, the full thickness of the aquifer will not be available for mixing of contaminants, and a lesser thickness may be derived from evidence of high permeability zones from borehole logs, annual water table fluctuation from hydrographs, or local experience. Many UK aquifers are layered systems with significant vertical heterogeneity that limits the potential for vertical mixing.

The data entry cells that need to be completed will be highlighted blue. All other data entry cells will be blacked-out. Data sources should be documented on the worksheet in the yellow cells.

The following list provides additional information on data required to derive Level 2 remedial targets:

➢ Infiltration, (Inf): amount of recharge passing through contaminated source zone. May be a combination of percolating precipitation, leakage from sewers and drains, and deliberate discharges to soakaway. Note that the required units are m/day, so rainfall data in mm/year will need to be converted to the required units.

➢ Area of contaminant source, (A): The plan area of the soil contamination should be entered. This area is not used in the calculation and is for information only.

➢ Length of contaminant source, (L): The length of the source parallel to the groundwater flow direction should be entered.

➢ Saturated aquifer thickness, (da): distance from the water table to the base of the saturated aquifer.

➢ Hydraulic conductivity, (K): of the saturated aquifer (used to calculate groundwater flow in the underlying aquifer).

➢ Hydraulic gradient, (i): gradient of the water table in the saturated aquifer.

➢ Width of site, (w): longest extent of the site perpendicular (at 90 degrees) to groundwater flow direction. This value is carried through to the level 3 assessment and is set as the width of the contaminant source (Sy).

➢ Mixing zone depth,(Mz): thickness of saturated aquifer immediately beneath the site in which contaminated recharge mixes with flowing groundwater.

➢ Background concentration of contaminant (C_U): in groundwater up hydraulic gradient of the site.

When all of the blue cells have been completed, click away on another cell and the remedial target will be calculated and reported in the grey cells at the bottom of the screen. Three values are reported:

1. The calculated dilution factor, (DF);
2. The calculated Level 2 remedial target for soil, as mg/kg, for comparison with total soil concentrations;
3. The calculated Level 2 remedial target for soil, as mg/l, for comparison with leachability test results.

If the concentration of soil leachate is known, it is also possible to predict the impact on groundwater after dilution has occurred.

4.5 Level 3 Soil worksheet

The Level 3 Soil worksheet (Figure 4.4) is the final worksheet for assessing soil remedial targets in this package. It builds on the results of Level 1 and Level 2 soils worksheets, but additionally calculates the effects of advection and attenuation within the saturated aquifer.
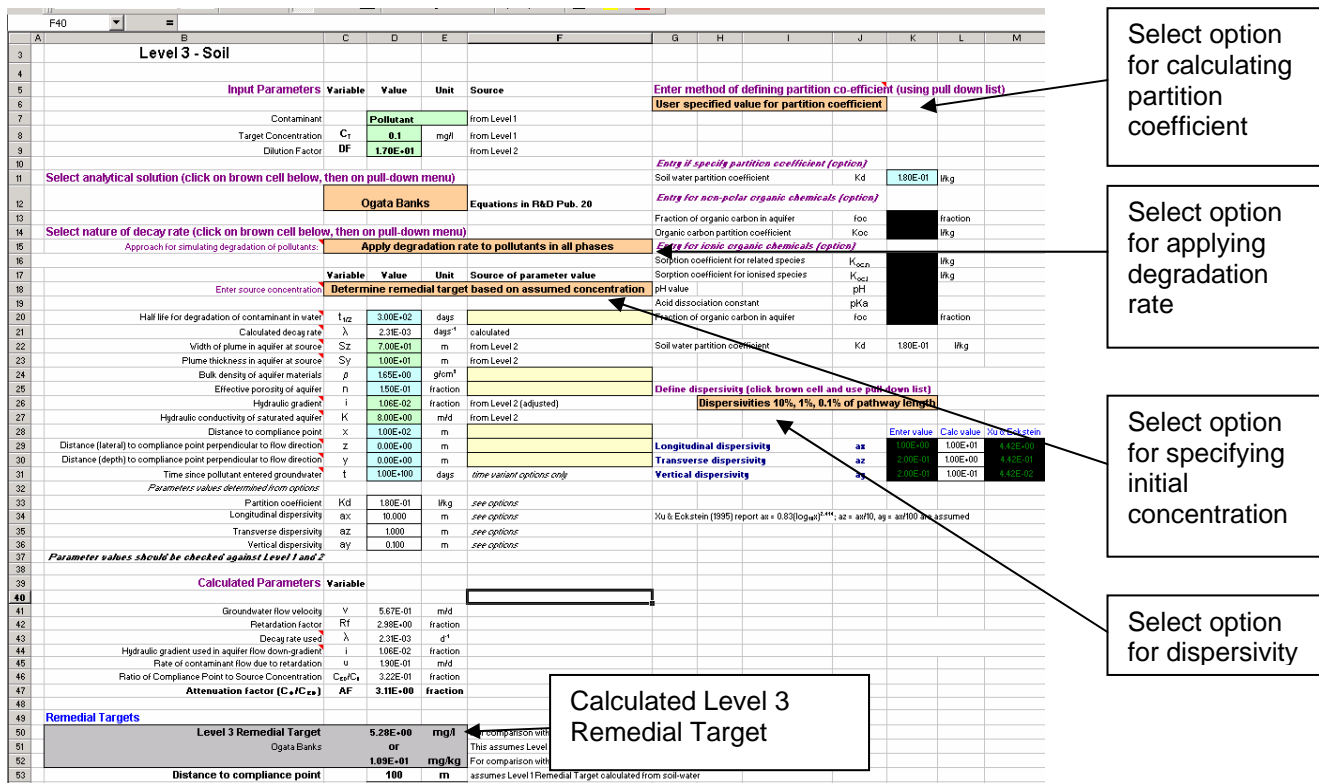
Figure 4.4   Level 3 Soil worksheet

Data on site details are transferred directly from the Introduction worksheet.
The dilution factor, DF, is transferred directly from the Level 2 soil worksheet.

Brown cells: There are four brown cells on the Level 3 Soil worksheet that need to be completed first in order to select the approach to simulating contaminant fate and transport. The following options are available:

1. Analytical solutions for contaminant transport:
    - Ogata Banks solution
    - Steady-state Domenico solution
    - Time-variant Domenico solution

2. Approach to modelling degradation processes:
    - First order biodegradation (degradation rate applied to contaminants in the dissolved phase only)
    - First order biodegradation or radioactive decay (degradation rate applied to contaminant in both dissolved and sorbed phases)

3. Option for specifying initial concentration (C_0):
    - Use soil leaching concentration
    - Use soil concentration to calculate soil pore water concentration
    - Use unit concentration (the calculation of the attenuation factor is based on the ratio of the initial concentration to the calculated concentration at the

compliance point and consequently the calculated remedial target is independent of the initial concentration).

For the first two options the spreadsheet will calculate contaminant concentrations (C) in groundwater down hydraulic gradient of the site taking into account dilution and remedial target. For the third option the spreadsheet will calculate contaminant concentrations as a ratio C/C_0.

4. Approach to contaminant partitioning between the aquifer matrix and groundwater:
    - User defined partition co-efficient
    - Calculate Kd on basis of non-polar organic species
    - Calculate Kd for polar organic species

5. Approach to modelling dispersivity within the aquifer:
    - User defined dispersivity values
    - Calculated dispersivity based on length of flowpath
    - Calculated dispersivity following empirical relationship derived by Xu & Eckstein (1995)

The options included within the worksheet solve the analytical solutions given below (please refer to *Remedial Target Methodology* for keys to parameters). It should be noted that the default solutions used to calculate remedial targets in 'Level 3 Soil' assume vertical dispersion in only one direction. This is consistent with the conceptual model of a soil source leaching down to the water table, and then dispersing within the aquifer. However, solutions using two directional vertical dispersion are presented in the calculation sheets, should this be more representative of the situation on a site.

Ogata Banks equation (vertical dispersion in one direction)

$$C_{ED} = \frac{C_0}{8} \exp\left\{ \frac{x}{2a_x}\left(1 - \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right) \right\} . erfc\left\{ \frac{1}{2\sqrt{a_x ut}} . \left(x - ut\sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right) \right\}$$

$$+ \exp\left\{ \frac{x}{2a_x}\left(1 + \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right) \right\} . erfc\left\{ \frac{1}{2\sqrt{a_x ut}} . \left(x + ut\sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right) \right\}$$

$$. \left[erf\left\{ \frac{z + \frac{S_z}{2}}{2\sqrt{a_z x}} \right\} - erf\left\{ \frac{z - \frac{S_z}{2}}{2\sqrt{a_z x}} \right\} \right] \left[erf\left\{ \frac{y + S_y}{2\sqrt{a_y x}} \right\} - erf\left\{ \frac{y - S_y}{2\sqrt{a_y x}} \right\} \right]$$

Ogata Banks equation (vertical dispersion in two directions)

$$C_{ED} = \frac{C_0}{8} \exp\left\{\frac{x}{2a_x}\left(1 - \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x - ut\sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}$$

$$+ \exp\left\{\frac{x}{2a_x}\left(1 + \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x + ut\sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}$$

$$\cdot\left[erf\left\{\frac{z + \frac{S_z}{2}}{2\sqrt{a_z x}}\right\} - erf\left\{\frac{z - \frac{S_z}{2}}{2\sqrt{a_z x}}\right\}\right]\left[erf\left\{\frac{y + \frac{S_y}{2}}{2\sqrt{a_y x}}\right\} - erf\left\{\frac{y - \frac{S_y}{2}}{2\sqrt{a_y x}}\right\}\right]$$

Steady state Domenico equation (vertical dispersion in one direction)

$$C_{ED} = C_0 \exp\left\{\frac{x}{2a_x}\left(1 - \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erf\left\{\frac{S_y}{2\sqrt{a_y x}}\right\}.erf\left\{\frac{S_z}{4\sqrt{a_z x}}\right\}$$

Steady state Domenico equation (vertical dispersion in two directions)

$$C_{ED} = C_0 \exp\left\{\frac{x}{2a_x}\left(1 - \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erf\left\{\frac{S_y}{4\sqrt{a_y x}}\right\}.erf\left\{\frac{S_z}{4\sqrt{a_z x}}\right\}$$

Time variant Domenico equation (vertical dispersion in one direction)

$$C_{ED} = \frac{C_0}{2} \exp\left\{\frac{x}{2a_x}\left(1 - \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x - ut\sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erf\left\{\frac{S_y}{2\sqrt{a_y x}}\right\}.erf\left\{\frac{S_z}{4\sqrt{a_z x}}\right\}$$

Time variant Domenico equation (vertical dispersion in two directions)

$$C_{ED} = \frac{C_0}{2} \exp\left\{\frac{x}{2a_x}\left(1 - \sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x - ut\sqrt{\left[1 + \frac{4\lambda a_x}{u}\right]}\right)\right\}.erf\left\{\frac{S_y}{4\sqrt{a_y x}}\right\}.erf\left\{\frac{S_z}{4\sqrt{a_z x}}\right\}$$

Important points to note in selecting which approach to adopt include:

- The Environment Agency's preferred analytical solution for calculating Level 3 remedial targets for pollutants subject to first-order biodegradation in a homogeneous aquifer, is the Ogata-Banks solution.

- Where an aquifer is strongly heterogeneous, consideration should be given to the appropriateness of any of the solutions.
- If a time-variant solution is used, the time should be set to 9.9E+99 when deriving remedial targets.
- The three analytical solutions employed all assume (as a default) that the source of pollution is located at the top of the aquifer and vertical dispersion is considered in only one direction (i.e. downwards). An alternative solution based on vertical dispersion in two directions (up and down) is also provided in the calculation sheets and could be used if the source is in the middle of the aquifer profile. In most situations contaminants will enter groundwater after percolation through the unsaturated zone and vertical dispersion in only one direction is applicable.
- It is generally assumed that biodegradation of organic contaminants only occurs in the dissolved phase (since to pass through the cell membrane of micro-organisms the molecule must first be in aqueous solution). The worksheet provides a pull down menu that allows the user to select one of:
  1. Apply degradation rate to dissolved pollutants only. This is applicable where the decay rate is obtained from laboratory observations of the contaminant in water. In this case the rate constant is corrected in the spreadsheet by dividing it by the retardation factor, R_f. This results in degradation in the dissolved phase only being considered.
  2. Apply degradation rate to pollutants in all phases. This is applicable to radioactive decay, where the degradation rate is derived from field observations (e.g. long-term monitoring of groundwater) or laboratory experiments have been undertake using groundwater and the aquifer matrix. In this case the decay rate is applied to the whole system.
- User defined K_d values must reflect the partitioning of contaminants between groundwater and the aquifer matrix. This value of K_d is likely to be different from that used in Level 1 to model partitioning between pore water and soils.
- Calculated K_d should be based on relevant data (e.g. f_{oc} values must relate to the aquifer materials, and will therefore require different data from Level 1 assessments).
- Values for dispersivity of contaminants in the aquifer can either be calculated from one of two equations or user defined values can be entered as follows:

  1. Calculated bases on flow path length:

     Longitudinal dispersivity, a_x, based on 0.1 × flow path length

     Transverse dispersivity, a_z, based on 0.01 × flow path length

     Vertical dispersivity, a_y, based on 0.001 × flow path length

  2. Calculated using a solution derived by Xu and Eckstein (1995) where:

     $$a_x = 0.83(\log x)^{2.414}$$

     a_z and a_y are subsequently assumed to be 0.01 and 0.001 times the longitudinal dispersivity.

  3. User defined values for dispersivity may be obtained from tracer testing or experience of local hydrogeological conditions.

Blue cells: Having selected which approaches to modelling contaminant fate and transport are appropriate, it is necessary to populate the highlighted blue cells. **It should be remembered that data input on the Level 3 worksheet relates to behaviour of contaminants within the saturated aquifer. Physico-chemical data should be relevant to the aquifer matrix and are likely to be different from data input at Level 1 where the fate of contaminants in the 'soil' zone was modelled**. The following list identifies important issues related to each datum required:

➢ Half-life for degradation, $(t_{1/2})$: Contaminant decay is modelled as a first order reaction and degradation is defined by a half-life expressed in days. The worksheet gives the option to model biodegradation of dissolved phase only (where data are from laboratory analysis of degradation in water) or for the whole system (where data are from field observations or column tests, and are corrected to remove the effects of dispersion and retardation). If radioactive decay occurs, it may be assumed that this decay occurs irrespective of the phase in which the contaminant is located (i.e. in both the sorbed and dissolved phases).

➢ Decay rates should be based on field observation of contaminant destruction in groundwater, or on conservative literature values where their application is supported by field data. Any literature values used must relate to the behaviour of the chemical under similar environmental conditions (e.g. redox, pH, contaminant concentrations, presence of other substances etc). Guidance on assessing contaminant attenuation is given in Environment Agency R&D Publication 95 *Guidance on the assessment and monitoring of natural attenuation of contaminants in groundwater* (Environment Agency, 2000). Where contaminants are being assessed that are not subject to degradation, such as heavy metals (non-radioisotopes) and chloride, or there is no evidence of degradation from field data, a half-life of 9.9E+99 years should be used. A degradation rate of zero equates to a substance that degrades instantaneously.

➢ Width of source, (Sz): The width of the pollutant plume in the aquifer at the source (i.e. below the contaminated site) normal (at 90 degrees) to groundwater flow should be entered. This value is carried forward from the Level 2 worksheet and can only be changed in the Level 2 worksheet.

➢ Plume thickness at source, (Sy): The thickness of the pollutant plume in the aquifer at its source (i.e. below the contaminated site). The depth of the source is assumed to be equal to the mixing zone thickness, (M_z), used in Level 2 and this value is automatically carried forwards from the latter worksheet.

➢ Care should also be taken to ensure that the modelled effects of vertical dispersion are not so great as to simulate a plume that extends beyond the physical limits of the aquifer. If the worksheet calculates that the modelled effects of vertical dispersion are to spread the plume beyond the thickness of the aquifer unit, a warning will be posted that "*Dispersed plume thickness exceeds aquifer thickness! Reduce vertical dispersivity*". In this the value for vertical dispersivity should be reduced. This can only be achieved under option to enter dispersivity values.

➢ Dry Bulk density: of the aquifer material.

➤ Effective porosity, (n): of the aquifer - drainable pore space. In fissured and dual porosity aquifers, the effective porosity may be assumed to be the fissure porosity. This value applies to the saturated zone only and is not therefore the sum of the air and water filled porosities used in Level 1. The 'Porosity Calculator' worksheet should not be used to derive values of effective porosity.

➤ Hydraulic gradient, (i): gradient of the water table in the saturated aquifer. The hydraulic gradient is entered in the level 2 worksheet but is then corrected to ensure that groundwater fluxes up and down-gradient of the site balance. The correction is:

$$i_{level3} = i_{level2} \cdot \left\{ \frac{DF}{DF - 1} \right\}$$

➤ where DF is the Dilution Factor calculated at Level 2 using relative volumes of infiltration and groundwater flow. The corrected value for the hydraulic gradient is shown in a coloured light green box. This value cannot be changed in the level 3 worksheet and the hydraulic gradient can only be changed in the level 2 worksheet.

➤ Hydraulic conductivity, (K): of the aquifer in a water-saturated state. The hydraulic conductivity is entered in the level 2 worksheet and automatically transferred to the level 3 worksheet.

➤ Distance to compliance point, (x): the distance from the source to the point at which compliance with an environmental standard is required.

➤ Distance (lateral) to the compliance point, (z): the off-set distance of the compliance point or monitoring borehole from the groundwater/plume centreline of flow (Figure 4.5).
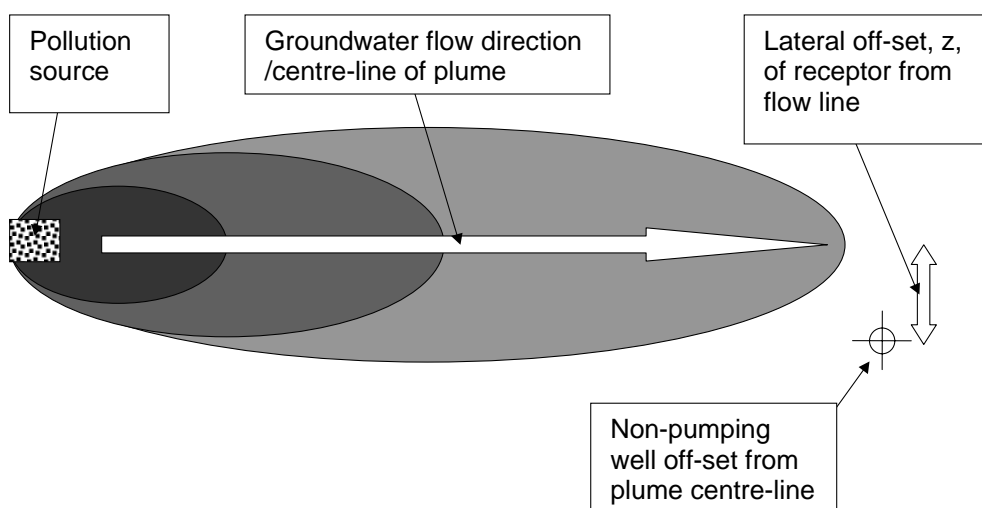

Figure 4.5 Lateral off-set, z, of compliance point from plume centre-line.

Distance (vertical) to the compliance point, (y): the vertical off-set distance of the compliance point or monitoring borehole from the groundwater/plume centreline of flow (Figure 4.6).
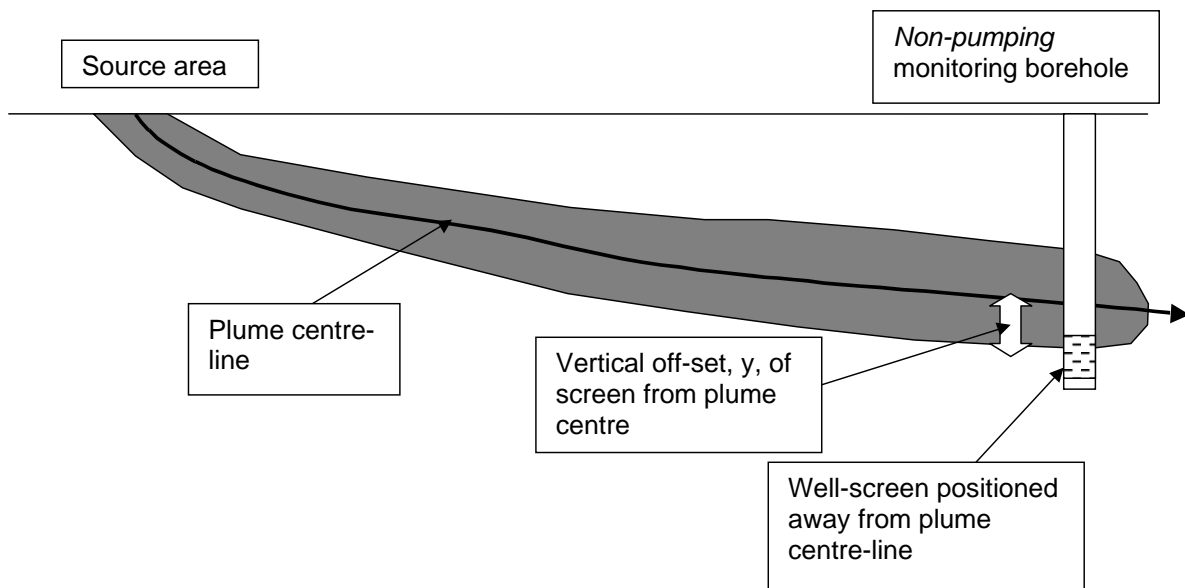

Figure 4.6 Vertical off-set, y, of receptor (well screen) from plume centre-line

The vertical and lateral distance to the compliance point should be set as zero in order to determine remedial target concentrations. Distances should only be entered where it is necessary to predict the concentration of a contaminant in a borehole that is offset from the plume centre line or to derive a trigger concentration for a compliance monitoring borehole.

➢ Time, (t): For time-variant assessments, the worksheet can be used to predict the contaminant fate at various times (e.g. to predict when a plume might reach a receptor or to predict the size of a plume after 10 years). When the worksheet is used to derive remedial targets, the time (in time-variant options) should be set to a very large number, such as 9.9E+99, in order to avoid overestimating the required remedial targets to protect receptors.

➢ Soil water partition coefficient: (K_d) values should relate to the partitioning of contaminants between groundwater and aquifer materials. For conservative contaminants, K_d equals zero.

➢ Fraction of organic carbon, (f_{oc}): value for the aquifer within which the plume is migrating. The foc value used should relate to the unpolluted aquifer material, and should not include organic pollutants that may be present in the aquifer.

➢ Organic carbon partition coefficient, (K_{oc}): Contaminant specific value, K_{oc}, which describes the partitioning of a substance between organic matter and water. An appropriate value must be inserted into the blue cell, if calculating K_d for non-polar ionic compounds.

➢ A conservative organic compound has a K_{oc} value of zero.

➤ pH and acid dissociation constants: contaminant specific data necessary to derive partition coefficients for polar organic substances.

Results

When each of the blue cells has been completed, click on another cell and the worksheet will calculate Level 3 remedial targets for soil and present the results in the grey box at the bottom of the screen. Remedial targets are presented as soil concentration (mg/kg) and leachable concentration (mg/l).

The spreadsheet also gives the calculated:
- groundwater velocity;
- retardation factor;
- rate of contaminant movement;
- decay rate
- ratio of contaminant concentration at compliance point to initial concentration
- Attenuation factor.

In addition the spreadsheet includes:
- Graph (Figure 4.7) showing variation in contaminant concentrations down-gradient of the source (expressed as C_0/C);
- Table giving calculated concentrations in groundwater between the source and the compliance point expressed as C_0/C and C (if starting concentration is entered);
- Graph (Figure 4.7) showing the predicted concentrations with distance from each of the three analytical solutions (located to the right of the main data input area).

Note: if a vertical or lateral offset is specified then the graph and table present contaminant concentrations along a line that is offset from the plume centre line.
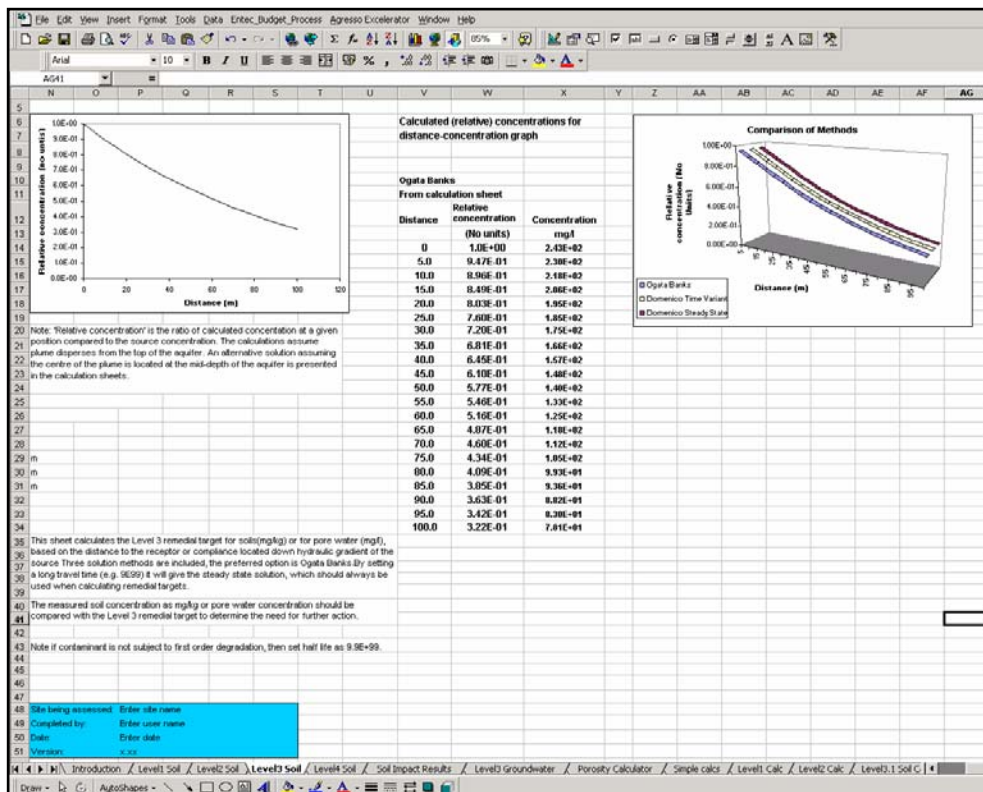
Figure 4.7 Comparison of contaminant behaviour predicted by analytical solutions.

4.6 Soil impact calculations worksheet

The soil impact calculation worksheet (Figure 4.8) presents the predicted impact on water quality (as a contaminant concentration) arising from a soil source, that are calculated at each of the three levels.

The spreadsheet allows the soil contaminant concentration (as mg/kg) to be entered and uses this to calculate:
• Pore water concentration;
• Contaminant concentration in groundwater below the source (due to dilution);
• Contaminant concentration at the compliance point.

The data needed for these calculations are automatically transferred from the Level 1 to 3 soil worksheets.

The worksheet also includes a figure and table that gives calculated concentrations in groundwater between the source and the compliance point.
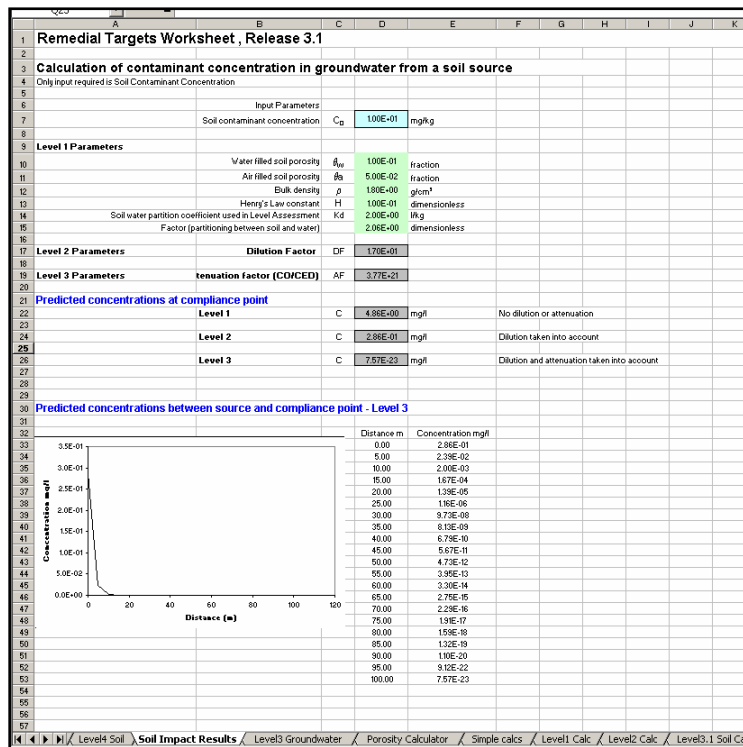
Figure 4.8 Soil impact calculation worksheet

4.7 Porosity calculator worksheet

The air and water filled porosities can be difficult parameters to measure directly at a site area, but can be estimated from soil bulk density (wet or dry), particle density and moisture content. The calculations presented in the 'Porosity Calculator' worksheet are suitable for inclusion within the Level 1 and 2 soil worksheets and for the Level 2 Vapour assessment.

If using dry bulk density data the formulae used within the model are as follows:

$$Void\_Ratio = \frac{Particle\_density}{Dry\_bulk\_density} - 1$$

$$Initial\_Saturation,\% = \frac{Moisture\_content * Particle\_density}{Void\_ratio}$$

$$Total\_porosity = 1 - \frac{Dry\_bulk\_density}{Particle\_density}$$

$$Air\_filled\_porosity = \frac{(100 - initial\_saturation) * total\_porosity}{100}$$

$$Water\_filled\_porosity = (total\_porosity) - (air\_filled\_porosity)$$

where:

porosities and void ratio are expressed as fractions
densities are expressed as g/cm^3
moisture content expressed as % by weight
initial saturation expressed as %

If using wet bulk density data the wet bulk density is converted to a dry bulk density using the following formula, then the air and water filled porosities are calculated using the formula above.

$$Dry\_bulk\_density = \frac{100 * wet\_bulk\_density}{100 + Moisture\_content}$$

It is important to note that these equations cannot be used to calculate the effective porosities used for the Level 3 Soil and Groundwater assessment worksheets.

4.8 Level 3 Groundwater worksheet

The Level 3 Groundwater worksheet (Figure 4.9) performs the same groundwater transport calculations as Level 3 Soil with the distinction that it does not require data from Levels 1 and 2 soil worksheets and simply models migration of contaminants within the aquifer.

Level 3 Groundwater worksheet does, however, offer the option to simulate contaminant transport with vertical dispersion in either one or two directions, depending whether the plume is located at the edge (top or bottom) or centre of the aquifer.

Data requirements for Level 3 Groundwater are similar to Level 3 Soil and are not described further. The exception is that the following values need to be entered:
• Contaminant concentration in groundwater;
• Hydraulic conductivity;
• Hydraulic gradient;
• Source width and depth.

The calculated remedial targets are restricted to a Level 3 remedial target for groundwater, expressed as mg/l, which should be compared to groundwater quality at the contaminated site.

The spreadsheet also includes:
• Graph showing the variation in contaminant concentrations downgradient of the source (expressed as mg/l);

- Table giving calculated concentrations in groundwater between the source and the compliance point (expressed as mg/l).
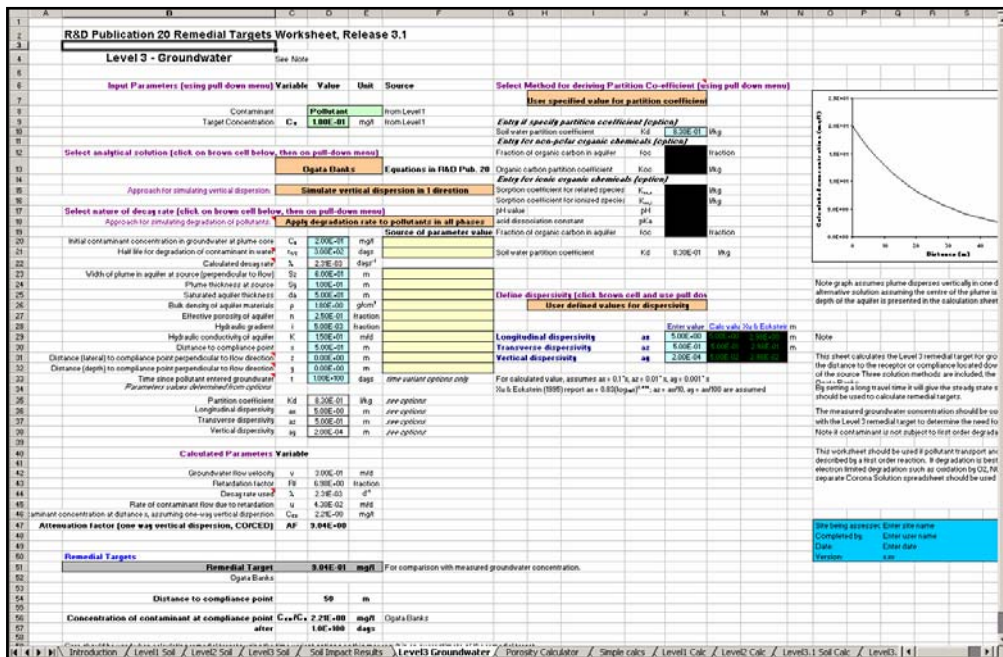

Figure 4.9 Level 3 Groundwater worksheet

Results

When each of the blue cells has been completed, click on another cell and the worksheet will calculate Level 3 remedial targets for groundwater and present the results in the grey box at the bottom of the screen. Remedial targets are presented as groundwater concentration (mg/l).

The spreadsheet also gives the calculated:
- Groundwater velocity
- Contaminant concentration at compliance point
- Attenuation factor.

In addition the spreadsheet includes:
- Graph showing variation in contaminant concentrations down-gradient of the source (expressed as mg/l) for both steady state and time variant solutions;
- Table giving calculated concentrations in groundwater between the source and the compliance point (expressed as mg/l) for both steady state and time variant solutions.

5 Sensitivity analysis

Each of the worksheets presented allows remedial targets to be calculated for a single contaminant at a time using a deterministic method, that is to say, a remedial target is calculated on the basis of a single parameter value for each variable. It is recommended that analysis of the sensitivity of the calculated remedial target to changes or variability in the input data is undertaken as part of the risk assessment process. Understanding how the magnitude of risks vary with changes in input parameter values in essential to understanding the certainty that can be placed on any prediction.

Two principal methods are available to take account of parameter uncertainty. A common method that allows parameter variability to be considered is the use of probabilistic methods, such as Monte Carlo analysis. This worksheet is password protected and this may prevent the use of common commercial tools, such as Crystal Ball™ and @Risk™, to undertake Monte Carlo analysis. If Monte Carlo analysis is required, it is recommended that an alternative assessment tool, such as ConSim (Environment Agency, 1999b) is used.

A second approach to assessing the effects of parameter variability on the calculated remedial targets is described in chapter 8 of the *Remedial Targets Methodology: Hydrogeological Risk Assessment for Land Contamination*. By varying selected input parameters in turn and observing the effect on the calculated remedial target it is possible to determine which parameters make the greatest effect on the results. Having assessed which parameters the calculations are most sensitive to, and considered the anticipated variability in parameter values, it is then possible to decide whether to revisit the assessment to collect more data on those parameter(s) to reduce uncertainty in the result. Alternatively it may be appropriate to adopt conservative values for those sensitive parameters, in order to ensure that the calculated remedial targets are protective of the environment.

Further *guidance on assigning values to uncertain parameters in subsurface contaminant fate and transport modelling* is provided in Environment Agency (2001c).

6 Simple hydrogeological calculations worksheet

In addition to the remedial targets worksheets, a separate sheet titled 'Simple hydrogeological calculations' is included (Figure 6.1). This worksheet is not needed to complete any of the calculations described in the methodology, but computes a range of standard calculations that are frequently used by hydrogeologists.

Data requirements for each calculation are described in the comments boxes, noted by a red tick in the corner of relevant cells. The calculations performed are summarised below:

Calculation	Mathematical solution
Groundwater flow velocity	$v_{GW} = (K \times i) / n$
Time for GW to reach to receptor	$t_{GW} = (n \times distance) / (K \times i)$
Volume of GW flowing through aquifer	$Q = K \times A \times i$
Contaminant flow velocity	$v_{contam} = (K \times i) / (n \times R_f)$
Time for contaminant to reach receptor	$t_{contam} = (n \times R_f \times distance) / (K \times i)$
Retardation factor, R_f	$R_f = 1 + [(K_d \times \rho) / n]$

The results of each calculation are presented in a range of units for ease of interpretation.

Figure 6.1 Worksheet for simple hydrogeological calculations.

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