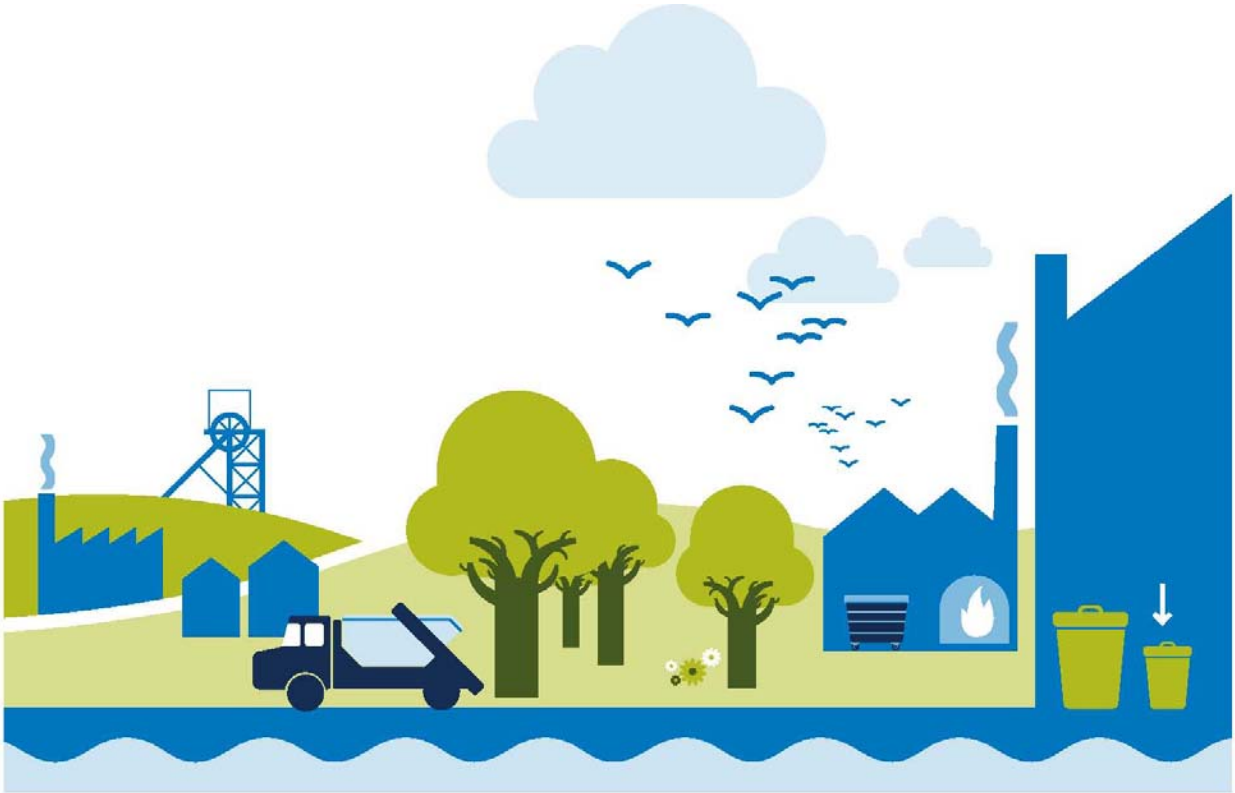
Horizontal Guidance H1 - Annex J 5: Infiltration Worksheet User Manual v1.2

Groundwater risk assessment for treated effluent discharges to infiltration systems



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Summary of changes

Below is a summary of changes made to this Annex since the launch in February 2011.

Annex version	Date	Change	Template version
Issue 1.2	November 2011	Reformatting to respond to general issues raised in the 2010 H1 public consultation. Minor review of text and layout.	H1 April 2011

Introduction

Infiltration Worksheet User Manual v1.2

We have prepared this User Manual to assist users of our Infiltration Worksheet v1.1. This document describes the functionality of the worksheet and gives guidance on its use.

The worksheet provides a means of carrying out some of the calculations behind the framework on *Annex J 4 Groundwater risk assessment for treated effluent discharges to infiltration systems* (Environment Agency, 2011a), which forms a technical annex to our H1 Environmental Risk Assessment*: Annex (j) groundwater* (Environment Agency, 2011b).

More general information on our approach to risk assessment and the underlying regulatory context and Environment Agency position are set out in the following documents:

- *Groundwater Protection: Policy and Practice (GP3) Parts 1-4* (Environment Agency, 2006 -2008)[1]
- *Guidelines for environmental risk assessment and management.* The Stationery Office (DETR *et al*, 2000).

We strongly recommended that you read and become familiar with the relevant sections of these documents before using the Infiltration Worksheet.

Specifically, we have developed the Infiltration Worksheet to help determine the risk to groundwater from discharges of treated effluent via infiltration systems (such as a drainage field designed to British Standards) and it should only be used in this context.

The worksheet should only be used by suitably experienced hydrogeologists or those fully conversant with our approach to groundwater risk assessment and the relevant England and Wales legislation and guidance.

Obtaining and installing the worksheet

You can download the worksheet from our H1 Environmental Risk Assessment website.

We have prepared and tested the Worksheet in Microsoft Excel 2002™[2] on the Microsoft 95/2000/XP™ operating systems. The file comprises about 550 KB and should not require any significant additional computing capability beyond that needed to run Microsoft Excel 2002™.

[1] An update of GP3 including a new Part 5 is planned for launch in 2012.

[2] The worksheet is currently being tested for use on later versions of Microsoft Excel™ and other Microsoft™ operating systems

We recommend that a blank copy of the worksheet is saved as a master file and that each simulation is saved as a distinct file.

In order to enable the worksheet, a number of capabilities are required in Microsoft Excel 2002™ that may not automatically be set. The worksheet calculates error functions and complimentary error functions. Before using the worksheet, you will need to add these capabilities by clicking the following from the pull-down Tools menu:

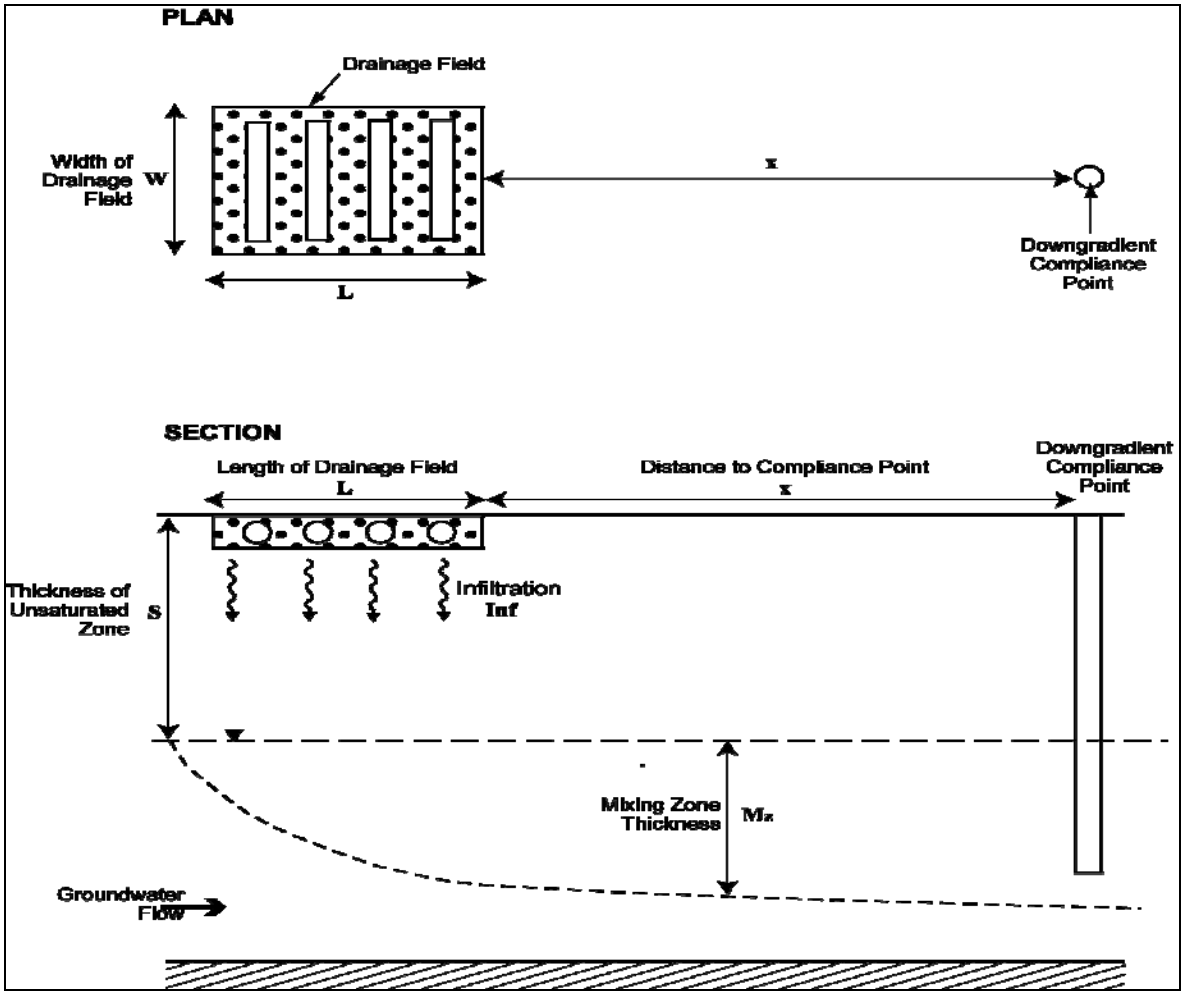
Tools ⇒**Add-Ins** ⇒ **Analysis ToolPak** *and* **Analysis ToolPak-VBA**.

You must also **Enable Macros** when prompted to do so upon opening up the worksheet.

1.0 Overview

An illustration of a typical setting for which the Infiltration Worksheet could be used is given in Figure 1.1

Figure 1.1 Discharge of treated effluent to infiltration systems and the application of the Infiltration Worksheet



You can use the spreadsheet to:

- calculate the area of the drainage field;
- calculate the average infiltration rate over the drainage field;
- determine attenuation within the unsaturated zone and calculate the concentration of the substance of concern at the water table;

- determine the dilution factor for non-hazardous pollutants and calculate their concentration in groundwater immediately down-gradient of the drainage field;
- determine attenuation within the saturated zone for non-hazardous pollutants and calculate their concentration at a point down-gradient of the drainage field; and
- determine provisional discharge limit values.

Box 1.1 contains a definition of some of the main terms used in this User Manual.

Box 1.1 Definition of standard terms

Term	Definition
Compliance point	A compliance point is a suitable point along the substance pathway between the source and a receptor at which a compliance value can be set. The compliance point may be a virtual point (for the purpose of predictive assessments) or it may be a physical monitoring point such as a borehole. In some cases the compliance point may be the receptor itself.
Compliance value	This is a concentration at the compliance point that should not be exceeded. Depending on the level of assessment, a compliance value may take account of some or all of the dilution and attenuation processes along the substance pathway to the receptor(s). The purpose of the selected compliance value is to provide protection to a down-gradient receptor – provided the compliance value is met the relevant environmental standard for the receptor(s) should also be met.
Discharge limit value	A discharge limit value is a value set as a condition in the permit to control a specified substance in the discharge with the aim of preventing the input of hazardous substances to groundwater or pollution due to the input of non-hazardous pollutants.
Dilution factor	The dilution factor describes the amount of dilution of the discharge by groundwater flow and is calculated from the ratio of groundwater below the drainage field and the discharge to the drainage field.
Attenuation factor (unsaturated zone)	The attenuation factor in the unsaturated zone can be calculated as the ratio between the concentration of the substance in the treated effluent and the predicted concentration at the base of the unsaturated zone.
Attenuation factor (saturated zone)	The attenuation factor in the saturated zone can be calculated as the ratio between the concentration of the substance in groundwater below the drainage field and the predicted concentration at a point down-gradient of the drainage field.

Box 1.1 continued

Term	Definition
Environmental standard	The environmental standard used to derive the compliance values will depend on (a) whether the substance is a hazardous substance or a non-hazardous pollutant and (b) the use of the receptor (for example, a potable abstraction or surface water). Examples of environmental standards are: • **Limits of detection** or where applicable a **Minimum Reporting Value** (MRV), MRVs are typically used to assess the discernibility of hazardous substances as a basis for deciding whether their input has been prevented; • **Natural background (up-gradient) quality**. This might be used to assess the discernibility of hazardous substances where background concentrations are higher than detection limits or the MRV. Alternatively it might be used for non-hazardous pollutants where the natural background concentration exceeds the relevant standard such as a drinking water standard (DWS) or environmental quality standard (EQS). **DWS (Drinking Water Standard) or EQS (Environmental Quality Standard).** In some cases it will be appropriate to use lower concentrations than the DWS or EQS to provide satisfactory protection to a receptor. For example, it may be suitable to apply a safety factor to provide greater security to an existing drinking water supply (such as 0.75 x DWS). In other cases where the DWS or EQS represents a significantly higher concentration than the natural background quality, use of such values might represent a significant level of deterioration (for example, a DWS of 250 mg/l of chloride compared to a background concentration of for example, 30 mg/l). In these cases you may need to discuss this with us and derive a more suitable value between the MRV or background concentration and the EQS or DWS.

2.0 The risk assessment approach and the site conceptual model.

The tools selected to model a site should be appropriate to the conceptual model and the quality of the available data. Guidance on these issues is provided in:

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

You should only employ the Infiltration Worksheet where a robust conceptual model has been developed and you are satisfied that the calculations performed by the worksheet are relevant to the processes described within that conceptual model.

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.

Your conceptual model should be supported by valid data. Good quality site specific data is always preferred. If you use generic data it should be reliable and relevant to the site. You should document the provenance and relevance of all data included in an assessment using the worksheet and include this in any report(s) submitted to us for consideration. The Infiltration Worksheet should only be used when adequate site-specific data have been obtained. For further guidance on sources of information and which site-specific data are required the reader should refer to Environment Agency (2011a and 2011b).

The following guidance on reviewing assessments may also be of use in preparing reports for submission as part of any application:

- *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 (Environment Agency, 2001c).

2.1 Discharge limit values

Box 2.1 contains a summary of the basic calculations to determine the concentration of a substance at different points along the contaminant pathway (Figure 1.1). Box 2.2 illustrates how the discharge limit values are derived.

Box 2.1 Summary calculations for determining the concentration at different compliance points

Concentration at compliance point.

The concentrations of substances at different points along the pathway can be calculated as follows:

(i) Water table (*attenuation in unsaturated zone only)*:

$$C_{wt} = C_e / AF_u \qquad \text{(Equation 1)}$$

(ii) Borehole adjacent to infiltration system (attenuation in unsaturated zone and dilution)

$$C_{gw} = C_e / (AF_u \,.\, DF) \qquad \text{(Equation 2)}$$

(iii) Down-gradient borehole (attenuation in unsaturated and saturated zone and dilution - non hazardous pollutants only)

$$C_{dcp} = C_e / (AF_u \,.\, AF_s \,.\, DF) \qquad \text{(Equation 3)}$$

where:

C_{dcp}= Concentration at down-gradient compliance point (mg/l). Concentration should be below compliance value

C_{gw} = Concentration immediately down-gradient of drainage field point (mg/l)

C_{wt} = Concentration at base of unsaturated zone (mg/l)

C_e = Concentration of substance in treated effluent discharge (mg/l)

AF_u = Attenuation factor (unsaturated zone)

DF = Dilution factor

AF_s = Attenuation factor (saturated zone)

Box 2.2 Discharge limit values

Discharge limit values (*DCL*) can be calculated as follows:

(i) Attenuation in unsaturated zone only:

$$DCL_1 = AF_u \,.\, C_c \qquad \text{Equation 4)}$$

(ii) Attenuation in unsaturated zone and dilution

$$DCL_2 = DF \,.\, DCL_1 \qquad \text{(Equation 5)}$$

(iii) Attenuation in unsaturated and saturated zone and dilution (non hazardous pollutants only)

$$DCL_3 = AF_s \,.\, DCL_2 \qquad \text{(Equation 6)}$$

Where,

$DCL_{1\text{-}3}$ = Discharge limit value (these will vary depending on whether compliance point is: (DCL_1) base of unsaturated zone; (DCL_2) groundwater immediately down-gradient of drainage field; (DCL_3) groundwater down-gradient of drainage field.

DF = Dilution factor

AF_u = Attenuation factor (unsaturated zone)

AF_s = Attenuation factor (saturated zone)

C_c = Compliance value (mg/l) (for example, water quality standard or MRV)

You should regard any discharge limit values that are calculated using the worksheet as provisional. We may need to take additional information (such as, variability of leachate quality, type of treatment process, and assumptions in choice of parameter values) into account in defining the discharge limit values that will be specified as part of the environmental permit.

3.0 Using the worksheets

3.1 General

The Infiltration Worksheet v1.1 incorporates 10 sheets, which have the following functions:

Table 3.1 Function of worksheets

Title of worksheet	Function of worksheet
Introduction	Brief instructions, entry of site details, assessor details, substance and environmental standard used (and its origin) to derive the compliance value for transfer to subsequent sheets
Infiltration System	Data entry for infiltration system including infiltration rate and area of drainage field
Attenuation_unsatzone	Data entry for calculating attenuation in the unsaturated zone
Dilution	Data entry for calculating dilution factor and substance concentration in groundwater immediately down-gradient of the drainage field
Attenuation_satzone	Data entry for calculating attenuation factor in the saturated zone and substance concentration in groundwater down-gradient of the drainage field
Summary	Summary of results of calculations of impact of the discharge on groundwater and provisional discharge limit values
Additional calculations	Data entry and computation of simple hydrogeological calculations
Ammonium calculator	Data entry and conversion for different laboratory analysis of ammonium
Porosity calculator	Data entry and calculation of water-filled porosities
Attenuation calc_sat_zone	Calculation of attenuation factor in the saturated zone

Data entry is only possible in eight of the worksheets (as highlighted in blue in Table 3.1). Each of these eight worksheets also presents the results of each calculation. The calculations themselves are carried out in the remaining worksheets which are provided so that you can follow the mathematical calculations more easily. It is neither possible, nor necessary, to modify or enter data into any of the calculation sheets.

Each worksheet is password protected and data may only be entered in specific cells. The cells are colour-coded as detailed in Table 3.2.

Table 3.2 Colour scheme for the worksheets

	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
	Yellow cells should be used to record the origin or source of any data used in the worksheet. Although failure to populate the 'Source of parameter value' cells with appropriate text will not affect the spreadsheet calculations, it is good practice to complete this task. We will expect submitted reports to include these details
	Grey cells contain the results of each simulation
	Green cells contain information derived from another part of the worksheet

If you move the cursor over the red triangles at the corner of certain cells, further information is revealed on the data required or equations solved. Please also refer to Figure 3.2. Hyperlinks are provided in some of the worksheets.

3.2 Introduction worksheet

When starting a new assessment, you **MUST** complete details on the Introduction worksheet first (Figure 3.1). 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 substance;
- environmental standard used to derive the compliance value; and
- basis for environmental standard (for example, EQS, DWS, MRV, background quality).

You must complete all blue cells on the Introduction worksheet before moving onto any other worksheets. Data entered for the substance name, environmental standard, 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 cannot be amended within the subsequent worksheets, and can only be modified by changing the entry on the Introduction worksheet.

The Introduction worksheet also includes brief instructions on the use of the worksheet and a reminder that Microsoft Excel 2002™ Tools must be enabled to allow it to calculate error functions and complimentary error functions. The worksheet will not calculate attenuation factors, unless Microsoft Excel™ is set-up to calculate these mathematical functions.

It is necessary to undertake a separate simulation for each substance in the treated effluent.

You can find guidance on selecting an appropriate environmental standard, which are typically based on background water quality, Minimum Reporting Values (MRVs), drinking water standards (DWS) or environmental quality standards (EQS), in Environment Agency 2011a and 2011b.. See also Box 1.1.

Figure 3.1 Data entry required on Infiltration Introduction Worksheet

Details to be completed for each assessment				
Site Name:	Enter site name			
Site Address:	Enter site address			
Completed by:	Enter user name			
Date:	Enter date		Version:	x.xx
Substance	Chemical			
Environmental Standard (C_T)	0	mg/l	Origin of C_T:	Specify basis for standard (e.g. MRV, EQS, DWS)

3.3 Infiltration System worksheet

The Infiltration System worksheet (Figure 3.2) allows you to specify the concentration of the substance in the treated effluent and to enter details of the infiltration system.

Project information data (site and pollutant details) are automatically transferred to this worksheet from the Introduction worksheet.

The Infiltration System worksheet provides the following options (brown cells):

1. Specify the type of treatment plant. Four options are provided:

1. Septic tank.
2. Package treatment plant.
3. Treatment plant.
4. Other.

For septic tanks and package treatment plants you can input the following information:

- *Number of persons (p)*. Number of individuals served by the system. This information is used to calculate total discharge and the area of the drainage field.
- *Water use (litres/person/day).* Typical rates of sewage generation (in litres per person per day) are given in Environment Agency 2011a.
- *Percolation rate (Vp).* The percolation rate should be taken from percolation tests undertaken according to BS6297:2007 + A1:2008. This rate is used together with the number of persons to calculate the area of the drainage field (See Box 3.1).

2. Discharge rate. Two options are provided:

1. Enter the discharge rate
2. Calculate discharge rate (this option is only available for septic tanks and package treatment plants (see Box 3.1).

3. Area of drainage field. Two options are provided:

1. Enter the area of the drainage field.
2. Calculated area of the drainage field (this option is only available for septic tanks and package treatment plants (see Box 3.1).

A summary of the data requirements (blue cells) for this worksheet is given in Table 3.3. Depending on the options selected the worksheet will automatically grey out cells for which data entry is not required.

The Infiltration System worksheet calculates the following results:

- **Discharge rate** (**m^3/day)** based on the number of persons and water use (this option is only available for septic tanks and package treatment plants);
- **Area of the drainage field (m^2)** based on the number of persons and percolation rate derived from testing (this option is only available for septic tanks and package treatment plants);
- **Infiltration rate (m/day)** over the discharge area. This rate is used in subsequent calculations.

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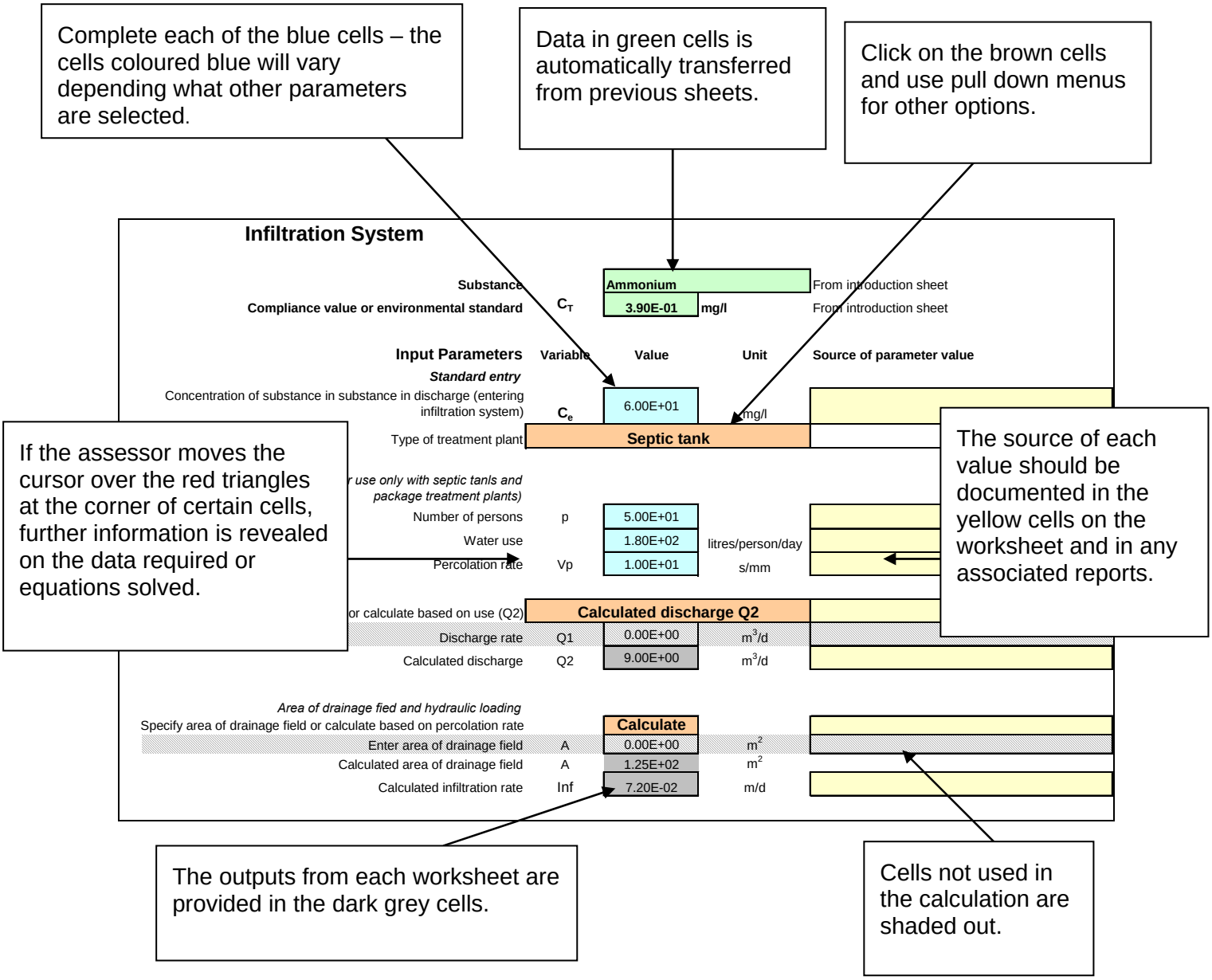


Figure 3.2 Examples of the main functionality on the worksheet. The Infiltration System worksheet (which has been used as an example here) calculates the discharge and infiltration rates. It can also calculate the Area of the Drainage Field (depending on what option is selected).

Box 3.1 Standard equations for the Infiltration System worksheet

The **hydraulic loading or infiltration rate (Inf)** is calculated from:

$$Inf = \frac{Q}{A} \qquad \text{(Equation 1)}$$

where:

Inf = Infiltration rate through the infiltration system (m/d)

Q = discharge rate to drainage field (m^3/d).

A = area of drainage field (m^2) (see below)

Note: The infiltration rate (*Inf*) should not exceed the maximum infiltration rate from BS 6297:2007 + A1:2008. This would indicate re-design of the drainage field was necessary. For some infiltration systems the design may include for storage to deal with peak flows, in these cases the infiltration rate should be set as the maximum infiltration rate.

The **discharge rate (Q)** is calculated as follows:

$$Q = p \,.W \qquad \text{(x 1 000: } m^3\text{/day to litres)} \qquad \text{(Equation 2)}$$

where:

Q = discharge rate to drainage field (m^3/d).

p = number of people served by the septic tank or package treatment plant

W = water use per person (litres/person/day)

The **area of a drainage field (A)** for domestic premises is calculated from (BS 6297:2007 + A1:2008):

$$A = (0.25)\,p.V_p \quad \text{for septic tanks} \qquad \text{(Equation 3)}$$

$$A = (0.20)\,p.V_p \quad \text{for package treatment plants} \qquad \text{(Equation 4)}$$

where:

A = area of drainage field (m^2)

p = number of people served by the septic tank or package treatment plant

V_p = percolation rate determined from percolation tests undertaken according to BS6297:2007 + A1:2008 (sec/mm)

Table 3.3 Summary of data requirements for the Infiltration System worksheet

Input parameter		Units	Comment	Other
Concentration of substance in treated effluent discharge	C_e	mg/l	Measured or taken from an agreed reference	Must be input
Number of persons	p		Number of people served by the septic tank or package treatment plant	Dependent on option selected
Water use		litres/person/day	Information on typical rates of sewage generation can be obtained from EA 2011a	
Percolation rate	V_p	sec/mm	Rate should be determined as set out in BS6297:2007 + A1:2008	
Discharge rate	Q_1	m^3/day	Measured or calculated based on number of persons or water use	Dependent on option selected
Area of drainage field	A	m^2	Measured or calculated based on number of persons and percolation rate	Dependent on option selected

3.4 Attenuation in Unsaturated Zone worksheet

The Attenuation in Unsaturated Zone worksheet (Figure 3.3) allows you to:

- calculate an attenuation factor (if degradation occurs) for the unsaturated zone;
- determine the concentration of the substance at the base of the unsaturated zone; and
- calculate a provisional discharge limit value. This limit may be superseded if dilution and attenuation in the saturated zone are taken into account.

Project information data (such as, site and substance details and infiltration rate) are automatically transferred to this worksheet.

The Attenuation in Unsaturated Zone worksheet provides the following options (brown cells):

1. Degradation. Three options are provided:

1. No degradation occurs. In this case the attenuation factor will be set as 1.

2. Degradation occurs in the dissolved phase only (degradation measured in the aqueous phase such as in aqueous laboratory experiments) and the user will need to enter a half life for degradation. This half life is likely to overestimate the rate of degradation in groundwater and therefore it is corrected by multiplying it by the retardation factor.

3. Degradation occurs in the dissolved and sorbed phase (degradation measured from field observations or laboratory experiments of the whole system that is both the dissolved and sorbed phases) and the user will need to enter a half life for degradation. This half life will be used in the calculation of an attenuation factor.

It is essential that you should be able to support the case for degradation. Please refer to Section 5.0. If no evidence for degradation is provided, you should select the option: 'No degradation occurs.'

2. **Soil-water partition coefficients**. Two options are provided:

1. Specify partition coefficient (typically used for inorganics such as metals and ammonium).

2. Calculate partition coefficient (non-polar organic substances only) based on fraction of organic carbon and organic carbon partition coefficient (see Box 3.2).

A summary of the data requirements (blue cells) for this worksheet is given in Table 3.3. Depending on the options selected, the worksheet will automatically grey out cells for which data entry is not required.

The worksheet will calculate the following (see also Box 3.2):

- **Attenuation factor** for the unsaturated zone;
- **Concentration of substance** at base of the unsaturated zone; and
- **Provisional discharge limit value** (DL_1).

Figure 3.3 Attenuation in Unsaturated Zone worksheet

Attenuation unsaturated zone

Contaminant		**Ammonium**		From introduction sheet
Compliance value or environmental standard	C_T	**3.90E-01**	mg/l	From introduction sheet
Concentration of substance in substance in discharge (entering infiltration system)	C_e	**6.00E+01**	mg/l	From infiltration sheet
Input Parameters	**Variable**	**Value**	**Unit**	**Source of parameter value**
Standard entry				
Infiltraton rate	**Inf**	**7.20E-02**	**m/d**	From infiltration sheet
Thickness of unsaturated zone below drainage field	S	1.50E+01	m	
Water filled porosity	□	1.00E-01	fraction	
Bulk density of unsaturated zone	□	1.80E+00	g/cm^3	
Calculated dispersivity	D	1.50E+00	m	calculated
Option to select degradation		**Degradation occurs - sorbed and dissolved phases**		
Half life for degradation of substance	$t_{1/2}$	3.65E+02	days	
Calculated decay rate	□…	1.90E-03	days^{-1}	calculated (very low value set if no degradation)
Fraction of rapid flow through unsaturated zone	□	0.00E+00	fraction	
Enter method of defining partition co-efficient (using pull down list)		**User specified value for partition coefficient**		
Entry if specify partition coefficient (option)				
Soil water partition coefficient	Kd	2.00E+00	l/kg	
Entry for organic chemicals (option)				
Fraction of organic carbon (in soil)	foc	1.00E-02	fraction	
Organic carbon partition coefficient	Koc	1.00E+01	l/kg	
Soil water partition coefficient used in assessment	**Kd**	**2.00E+00**	**l/kg**	*Specified value*
Retardation factor	Rfu	3.70E+01		
Unretarded travel time (no dispersion)	tu	2.08E+01	d	
Unretarded travel time (with dispersion)	tu	1.88E+01	d	
Retarded travel time (with dispersion)	tr	6.94E+02	d	
Attenuation factor	AFu	3.65E+00		

Attenuation factor and discharge consent limit

Unsaturated zone attenuation factor	**AFu**	**3.65E+00**	
Concentration at base of unsaturated zone	**C_{wt}**	**1.64E+01**	**mg/l**
		and	
Discharge limit value	**DL_1**	**1.43E+00**	**mg/l**

Additionally the worksheet will calculate:

- Dispersivity (taken as 10% of the thickness of the unsaturated zone);
- Decay rate for degradation;
- Soil-water partition coefficient (for non-polar organics);
- Retardation factor;
- Unretarded travel time of substance through unsaturated zone, with no dispersion;
- Unretarded and retarded travel time through the unsaturated zone, with dispersion.

A Summary of data requirements for the Attenuation in the Unsaturated Zone worksheet is provided in Table 3.3

Table 3.3 Summary of data requirements for the Attenuation in the Unsaturated Zone worksheet (blue cells)

Input parameter		Units	Comment	
Unsaturated zone thickness below the drainage field	S	m	Essential to have site specific measurement.	Must be input
Water filled porosity of the unsaturated zone	θ_w	fraction	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.	Must be input
Dry bulk density of unsaturated zone material	ρ	g/cm^3		Must be input
Half life for degradation of substance	$t_{1/2}$	$days^{-1}$	See Section 5.0.	Dependent on option selected
Percent rapid flow through the unsaturated zone	B	fraction	Set as 0 if no by-pass.	Must be input
Fraction of organic carbon for the unsaturated zone	foc		Expressed as a fraction between 0 and 1.	Must be input when non-polar organic chemicals option is selected
Organic carbon partition coefficient	Koc		Contaminant specific value which describes the partitioning of a substance between organic matter and water.	Must be input when non-polar organic chemicals option is selected

Input parameter		Units	Comment	
Soil water partition coefficient	Kd		Describes the partitioning of a substance between water and the soil matrix in the unsaturated zone. Soil water partition coefficients will typically be derived from literature sources, laboratory column experiments, or field data where comparison with a conservative tracer is possible. If a literature source is used it is important to ensure that it is relevant to the unsaturated zone material. For conservative contaminants the Kd value should be set at zero	Dependent on option selected

Box 3.2 gives an overview of the standard equations used in the Attenuation in the Unsaturated Zone worksheet.

Box 3.2 Standard equations for Attenuation in Unsaturated Zone worksheet

Decay rate (λ) is calculated from:

$$\lambda = \ln(2)/H \qquad \text{(Equation 1)}$$

where:

λ = unsaturated zone decay constant (d^{-1})

H = Half life for degradation of substance (d)

Vertical dispersivity (α) in the unsaturated zone is calculated from:

$$\alpha = 0.1.S \qquad \text{(Equation 2)}$$

S = thickness of unsaturated zone below the drainage field (m)

Soil-water partition coefficient (*Kd*) is calculated for non-polar organics from:

$$K_d = K_{oc}.f_{oc} \qquad \text{(Equation 3)}$$

where:

Koc = Organic carbon partition coefficient (l/kg)

foc = fraction of organic carbon

Box 3.2 continued

Retardation Factor in the unsaturated zone (*Rfu*) is calculated from:

$$Rfu = 1 + Kd.\rho/\theta_w \quad \text{(Equation 4)}$$

where:

θ_w = water filled porosity of unsaturated zone (fraction)

p = dry bulk density of unsaturated zone (g/cm^3)

The **unretarded travel time (*tu*)** through the unsaturated zone is calculated from:

$$tu = S.\theta / Inf \quad \text{(Equation 5)}$$

where:

Inf = Infiltration rate through the infiltration system (m/d)

The retarded travel time (*tr*) through the unsaturated zone is calculated from:

$$tr = tu.Rfu \quad \text{(Equation 6)}$$

The above calculation for unretarded travel times ignores dispersion; if dispersion is taken into account the travel time is calculated from:

$$tu = (S - \alpha).\theta / Inf \quad \text{(Equation 7)}$$

An **attenuation factor (AFu) for the unsaturated zone** can be calculated from:

$$AFu = 1/\exp\left[\frac{S}{2\alpha} - \left\{\frac{S}{2\alpha}\sqrt{1 + (4a\lambda/v_{ur})}\right\}\right] \quad \text{(Equation 8)}$$

where:

v_{ur} = retarded contaminant velocity in the unsaturated zone (m)

$$v_{ur} = (Inf / \theta_w)/R \quad \text{(Equation 9)}$$

a = longitudinal dispersivity

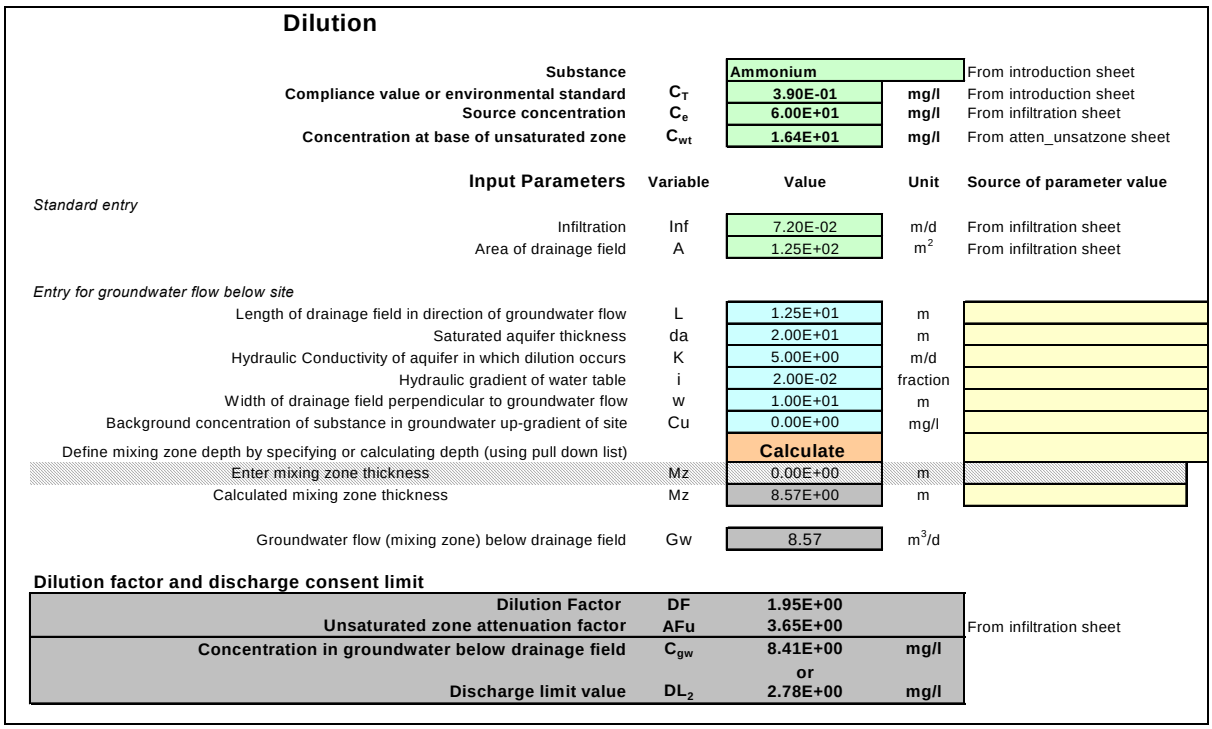
3.5 Dilution worksheet

The Dilution worksheet (Figure 3.4) allows users to:

- Calculate a dilution factor to account for dilution by groundwater flow below the drainage field (Box 3.3);
- Determine the concentration of the substance in groundwater immediately down-gradient of the drainage field; and
- calculate a provisional discharge limit value. This limit may be superseded if attenuation in the saturated zone is taken into account (Section 3.6).

Project information data (for example, site and substance details, and unsaturated zone attenuation factor) are automatically transferred to this worksheet.

Figure 3.4 Dilution worksheet



Dilution

Substance		**Ammonium**		From introduction sheet
Compliance value or environmental standard	**C_T**	**3.90E-01**	**mg/l**	From introduction sheet
Source concentration	**C_e**	**6.00E+01**	**mg/l**	From infiltration sheet
Concentration at base of unsaturated zone	**C_{wt}**	**1.64E+01**	**mg/l**	From atten_unsatzone sheet
Input Parameters	**Variable**	**Value**	**Unit**	**Source of parameter value**
Standard entry				
Infiltration	Inf	7.20E-02	m/d	From infiltration sheet
Area of drainage field	A	1.25E+02	m^2	From infiltration sheet
Entry for groundwater flow below site				
Length of drainage field in direction of groundwater flow	L	1.25E+01	m	
Saturated aquifer thickness	da	2.00E+01	m	
Hydraulic Conductivity of aquifer in which dilution occurs	K	5.00E+00	m/d	
Hydraulic gradient of water table	i	2.00E-02	fraction	
Width of drainage field perpendicular to groundwater flow	w	1.00E+01	m	
Background concentration of substance in groundwater up-gradient of site	Cu	0.00E+00	mg/l	
Define mixing zone depth by specifying or calculating depth (using pull down list)		**Calculate**		
Enter mixing zone thickness	Mz	0.00E+00	m	
Calculated mixing zone thickness	Mz	8.57E+00	m	
Groundwater flow (mixing zone) below drainage field	Gw	8.57	m^3/d	

Dilution factor and discharge consent limit

Dilution Factor	**DF**	**1.95E+00**		
Unsaturated zone attenuation factor	**AFu**	**3.65E+00**		From infiltration sheet
Concentration in groundwater below drainage field	**C_{gw}**	**8.41E+00**	**mg/l**	
		or		
Discharge limit value	**DL_2**	**2.78E+00**	**mg/l**	

The worksheet provides the following option (brown cells):

Mixing Zone thickness. Two options are provided:

1. Specify the thickness of the mixing zone.

2. Calculate thickness of the mixing zone (see Box 3.3).

A summary of the data requirements (blue cells) for this worksheet is given in Table 3.4. Depending on the options selected the worksheet will automatically grey out cells for which data entry is not required.

The Dilution worksheet will calculate the following (see Box 3.3):

- **Dilution factor**, to account for dilution by groundwater flow below the drainage field;
- **Concentration of substance** in groundwater immediately down-gradient of the drainage field; and
- **Provisional discharge limit value** (DL_2).

Box 3.3 Standard Equations for the Dilution worksheet

The **dilution factor (DF)** for groundwater below the drainage field can be calculated from:

$$DF = \frac{(G_w + Inf.A).C_t - (G_w.C_u)}{Inf.A.C_t} \quad \text{(Equation 1)}$$

and

$$G_w = K.i.w_d.M_z \quad \text{(Equation 2)}$$

where:

Gw = Groundwater flow (mixing zone) below drainage field (m^3/d)

K = hydraulic conductivity (m/day)

i = hydraulic gradient

w_d = width of disposal field perpendicular to flow direction (m)

M_z = mixing zone thickness (m)

Inf = infiltration rate (m/day)

A = area of drainage field (m^2)

C_t = Environmental standard used to derive compliance value (mg//l)

C_u = background concentration of substance in groundwater immediately up-gradient of discharge field (mg/l)

The **mixing zone thickness** can be calculated as follows:

$$M_z = \sqrt{0.0112L^2} + da\left[1 - \exp\left(\frac{-L.Inf}{K.i.da}\right)\right] \quad \text{(Equation 3)}$$

where:

L = length of drainage field parallel to groundwater flow (m)

da = aquifer thickness (m)

Table 3.4 Summary of data requirements for the Dilution worksheet (blue cells)

Input parameter		Units	Comment	
Length of drainage field in direction of groundwater flow	L	m		Must be input
Saturated aquifer thickness	da	m		Must be input
Hydraulic conductivity of aquifer in which dilution occurs	K	m/d		Must be input
Hydraulic gradient of water table	i	fraction		Must be input
Width of drainage field perpendicular to groundwater flow	w_d	m		Must be input
Background concentration of substance in groundwater up hydraulic gradient of the site	C_u	mg/l		Must be input
Mixing zone thickness of saturated aquifer below drainage field	M_z	m	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.	Dependent on option selected

3.6 Attenuation in the Saturated Zone worksheet

The Attenuation in Saturated Zone worksheet (Figure 3.5) allows users to:

- Calculate an attenuation factor for the saturated zone (if degradation occurs) (see Box 3.4);
- Determine the concentration of the substance at a compliance point located down-gradient of the drainage field (see Box 3.4); and
- Calculate a provisional discharge limit value (see Box 2.2).

Project information data (such as, site and substance details and dilution factor) are automatically transferred to this worksheet from the previous sheets (green cells).

The worksheet provides the following options (brown cells):

1 **Degradation**. Three options are provided:

1. No degradation occurs. In this case the attenuation factor will be set as 1.

2. Degradation occurs in the dissolved phase only (degradation measured in the aqueous phase such as in aqueous laboratory experiments) and the user will need to enter a half life for degradation. This half life is likely to overestimate the rate of degradation in groundwater and therefore it is corrected by multiplying it by the retardation factor.

3. Degradation occurs in the dissolved and sorbed phase (degradation measured from field observations or laboratory experiments of the whole system that is both the dissolved and sorbed phases) and the user will need to enter a half life for degradation. This half life will be used in the calculation of an attenuation factor.

It is essential that you should be able to support the case for degradation. Please refer to Section 5.0. If no evidence for degradation is provided, you should select the option: 'No degradation occurs.'

2 **Partition coefficients**. Two options are provided:

1. Specify partition coefficient (typically used for inorganics such as metals and ammonium).

2. Calculate partition coefficient (non-polar organic substances only) based on fraction of organic carbon and organic carbon partition coefficient (see Box 3.2).

3 **Dispersivity**. Three options are provided:

1. Enter user defined dispersivity values.

2. Calculate dispersivity based on length of flow path (see Box 3.4).

3. Calculate dispersivity using Xu and Eckstein (1995) (see Box 3.4).

4 **Time**. Two options are provided:

1. Steady state. Use this to determine discharge limit values.

2. Enter time. Use this to validate the assessment if monitoring data are available.

A summary of the data requirements (blue cells) for this worksheet is given in Table 3.5. Depending on the options selected the worksheet will automatically grey out cells for which data entry is not required.

3.7 Calculated parameters

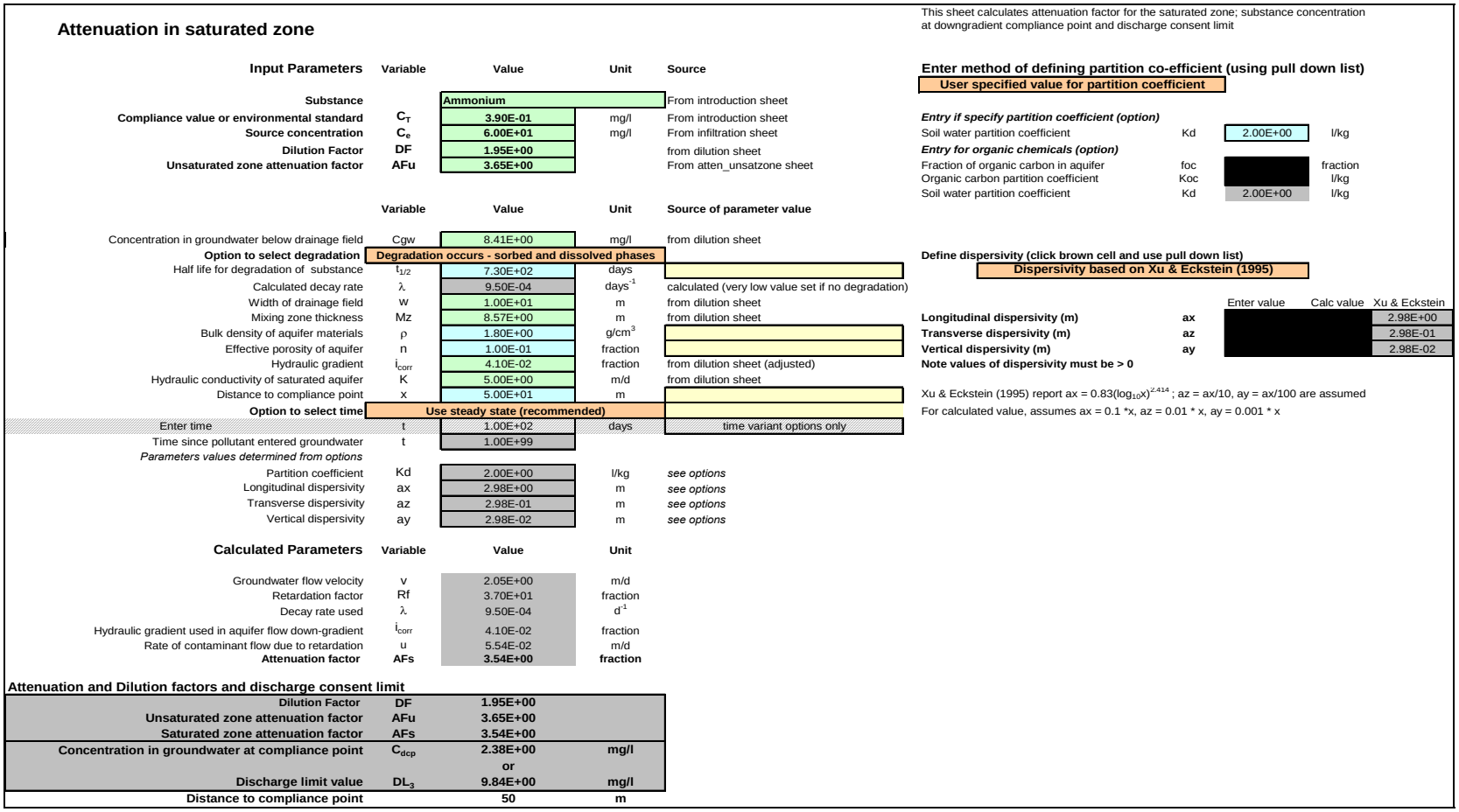
The Attenuation in the Saturated Zone worksheet will calculate the following:

- **Attenuation factor** for the saturated zone;
- **Concentration of substance** at a compliance point located down hydraulic gradient from the drainage field; and
- **Provisional discharge limit value** (DL_3).

Additionally:

- Decay rate for degradation;
- Hydraulic gradient (the hydraulic gradient entered in the previous worksheet is corrected to ensure that groundwater fluxes up and down-gradient of the drainage field balance);
- Soil-water partition coefficient (for non-polar organics);
- Retardation factor;
- Groundwater flow velocity and rate of contaminant flow due to retardation;
- Graph (Figure 3.6) showing variation in contaminant concentrations down-gradient of the source. It may be necessary to manually change the graph axes by clicking on the graph and selecting for format selected axes option (scale) in Excel; and
- Table giving calculated concentrations in groundwater between the source and the compliance point.

Infiltration Worksheet v1.2 User Manual



Attenuation in saturated zone

This sheet calculates attenuation factor for the saturated zone; substance concentration at downgradient compliance point and discharge consent limit

Input Parameters	Variable	Value	Unit	Source
Substance		**Ammonium**		From introduction sheet
Compliance value or environmental standard	**C_T**	**3.90E-01**	mg/l	From introduction sheet
Source concentration	**C_e**	**6.00E+01**	mg/l	From infiltration sheet
Dilution Factor	**DF**	**1.95E+00**		from dilution sheet
Unsaturated zone attenuation factor	**AFu**	**3.65E+00**		From atten_unsatzone sheet

	Variable	Value	Unit	Source of parameter value
Concentration in groundwater below drainage field	Cgw	8.41E+00	mg/l	from dilution sheet
Option to select degradation	**Degradation occurs - sorbed and dissolved phases**			
Half life for degradation of substance	$t_{1/2}$	7.30E+02	days	
Calculated decay rate	λ	9.50E-04	$days^{-1}$	calculated (very low value set if no degradation)
Width of drainage field	w	1.00E+01	m	from dilution sheet
Mixing zone thickness	Mz	8.57E+00	m	from dilution sheet
Bulk density of aquifer materials	ρ	1.80E+00	g/cm^3	
Effective porosity of aquifer	n	1.00E-01	fraction	
Hydraulic gradient	i_{corr}	4.10E-02	fraction	from dilution sheet (adjusted)
Hydraulic conductivity of saturated aquifer	K	5.00E+00	m/d	from dilution sheet
Distance to compliance point	x	5.00E+01	m	
Option to select time	**Use steady state (recommended)**			
Enter time	t	1.00E+02	days	time variant options only
Time since pollutant entered groundwater	t	1.00E+99		
Parameters values determined from options				
Partition coefficient	Kd	2.00E+00	l/kg	*see options*
Longitudinal dispersivity	ax	2.98E+00	m	*see options*
Transverse dispersivity	az	2.98E-01	m	*see options*
Vertical dispersivity	ay	2.98E-02	m	*see options*

Calculated Parameters	Variable	Value	Unit
Groundwater flow velocity	v	2.05E+00	m/d
Retardation factor	Rf	3.70E+01	fraction
Decay rate used	λ	9.50E-04	d^{-1}
Hydraulic gradient used in aquifer flow down-gradient	i_{corr}	4.10E-02	fraction
Rate of contaminant flow due to retardation	u	5.54E-02	m/d
Attenuation factor	**AFs**	**3.54E+00**	**fraction**

Attenuation and Dilution factors and discharge consent limit

Dilution Factor	**DF**	**1.95E+00**	
Unsaturated zone attenuation factor	**AFu**	**3.65E+00**	
Saturated zone attenuation factor	**AFs**	**3.54E+00**	
Concentration in groundwater at compliance point	**C_{dcp}**	**2.38E+00**	**mg/l**
		or	
Discharge limit value	**DL_3**	**9.84E+00**	**mg/l**
Distance to compliance point		**50**	**m**

Enter method of defining partition co-efficient (using pull down list)

User specified value for partition coefficient

Entry if specify partition coefficient (option)

Soil water partition coefficient — Kd — 2.00E+00 — l/kg

Entry for organic chemicals (option)

Fraction of organic carbon in aquifer — foc — fraction

Organic carbon partition coefficient — Koc — l/kg

Soil water partition coefficient — Kd — 2.00E+00 — l/kg

Define dispersivity (click brown cell and use pull down list)

Dispersivity based on Xu & Eckstein (1995)

		Enter value	Calc value	Xu & Eckstein
Longitudinal dispersivity (m)	**ax**			2.98E+00
Transverse dispersivity (m)	**az**			2.98E-01
Vertical dispersivity (m)	**ay**			2.98E-02

Note values of dispersivity must be > 0

Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x

Figure 3.5 Attenuation in Saturated Zone worksheet

Table 3.5 Summary of data requirements for Attenuation in Saturated Zone worksheet (blue cells)

Input parameter		Units	Comment	
Distance to compliance point	x	m	The distance from the source to the point at which compliance with an environmental standard is required.	Must be input
Effective porosity of the aquifer	θ_w	fraction	In fissured and dual porosity aquifers, the effective porosity may be assumed to be the fissure porosity.	Must be input
Dry Bulk density of the aquifer material	ρ	g/cm^3		Must be input
Half life for degradation of substance	$t_{1/2}$	days	See Section 5.0.	Dependent on option selected
Time	t	days	Time since substance entered groundwater.	Dependent on option selected
Soil water partition coefficient	K_d		Contaminant specific value, K_d, which describes the partitioning of a substance between the aquifer 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 substance is conservative (for example, it does not sorb to aquifer materials), the Kd value should be set to zero.	Dependent on option selected
Fraction of organic carbon	foc		Expressed as a fraction between 0 and 1.	
Organic carbon partition coefficient	Koc		Contaminant specific value which describes the partitioning of a substance between organic matter and water.	

Table 3.5 continued

Input parameter		Units	Comment	
Longitudinal, transverse and vertical dispersivity	a, a_y, a_z	m	Values for dispersivity may be obtained from tracer testing or experience of local hydrogeological conditions. A check should be undertaken to ensure that the modelled effects of vertical dispersion are not so great as to simulate a plume that extends beyond the base of the aquifer. The worksheet will post a warning if this occurs "*Dispersed plume thickness exceeds aquifer thickness! Reduce vertical dispersivity".* In these cases the value for vertical dispersivity should be reduced. This can only be achieved under the option to enter dispersivity values.	Dependent on option selected

Box 3.4 gives an overview of the equations used in the Attenuation in the Saturated Zone worksheet.

Box 3.4 Standard equations for Attenuation in Saturated Zone worksheet

Decay rate (λ) is calculated from:

$$\lambda = \ln(2)/H \qquad \text{(Equation 1)}$$

where:

λ = unsaturated zone decay constant (d^{-1})

H = t ½ (half life(days)

Soil water partition coefficient (*Kd*) is calculated from:

$$K_d = K_{oc} . f_{oc} \qquad \text{(Equation 2)}$$

where:

Koc = Organic carbon partition coefficient (l/kg)

foc = fraction of organic carbon of aquifer material

Retardation Factor (*Rf*) in the saturated zone is calculated from:

$$Rf = 1 + Kd.n/\rho \qquad \text{(Equation 3)}$$

where:

n = effective porosity of aquifer material (fraction) (if fissure porosity used the partition coefficient should be set as 0)

p = dry bulk density of aquifer (g/cm^3)

Values for dispersivity are calculated using either:

1. Xu and Eckstein

$$a_x = 0.83(\log x)^{2.414} \qquad \text{(Equation 4)}$$

$a_z = 0.01x$ and $a_y = 0.001x$ or

2.

$a_x = 0.1x$ and $a_z = 0.01x$ and $a_y = 0.001x$ (Equation 5)

where:

$\alpha_x, \alpha_z, \alpha_y$ = longitudinal, transversal and vertical dispersivity (m)

x = distance to down-gradient compliance point (m)

The worksheet **adjusts the hydraulic gradient (i)** as follows

$$i_{adjusted} = i.\left\{\frac{DF}{DF-1}\right\}$$

DF = dilution factor. (Equation 6)

This adjustment is undertaken to ensure that groundwater fluxes up and down-gradient of the drainage field balance

Box 3.4 continued

The **unretarded groundwater velocity** ***(v)*** through the saturated zone is calculated from:

$$v = K.i / n \qquad \text{(Equation 7)}$$

The **retarded groundwater velocity** *(u)* through the saturated zone is calculated from:

$$u = v / R \qquad \text{(Equation 8)}$$

K = hydraulic conductivity of aquifer in which dilution occurs (m/d)

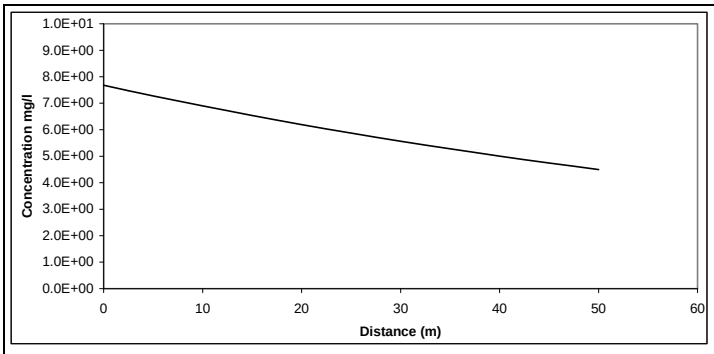
The **attenuation factor** ***(AFs)*** for the saturated zone is calculated from:

$$AFs = 8/\left\{\begin{array}{l}\exp\left\{\frac{x}{2a_x}\left(1-\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x-ut\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\} \\ +\exp\left\{\frac{x}{2a_x}\left(1+\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x+ut\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\} \\ .\left[erf\left\{\frac{z+\frac{S_z}{2}}{2\sqrt{a_z x}}\right\}-erf\left\{\frac{z-\frac{S_z}{2}}{2\sqrt{a_z x}}\right\}\right].\left[erf\left\{\frac{y+S_y}{2\sqrt{a_y x}}\right\}-erf\left\{\frac{y-S_y}{2\sqrt{a_y x}}\right\}\right]\end{array}\right\}$$

where:

erf and erfc are error function and complementary error functions respectively

Figure 3.6 Calculated concentrations in the Attenuation in the Saturated Zone worksheet



Calculated concentrations for distance-concentration graph

From calculation sheet

Distance m	Concentration mg/l
0	7.7E+00
2.5	7.48E+00
5.0	7.28E+00
7.5	7.09E+00
10.0	6.90E+00
12.5	6.72E+00
15.0	6.54E+00
17.5	6.37E+00
20.0	6.20E+00
22.5	6.03E+00
25.0	5.88E+00
27.5	5.72E+00
30.0	5.57E+00
32.5	5.42E+00
35.0	5.28E+00
37.5	5.14E+00
40.0	5.00E+00
42.5	4.87E+00
45.0	4.74E+00
47.5	4.62E+00
50.0	4.49E+00

3.8 Summary calculations worksheet

The Summary worksheet (Figure 3.7) requires no input as it presents data from previous worksheets and provides:

- A summary of compliance point data, dilution and attenuation factors;
- Calculated substance concentration at different points along the pathway (base of unsaturated zone, groundwater immediately down-gradient of drainage field, and groundwater down-gradient of the drainage field);
- Provisional discharge limit values for different points along the pathway.

The Summary worksheet also includes a chart that summarises calculated concentrations between the source and the down-gradient compliance point.

Figure 3.7 Summary calculations worksheet

Summary of calculations for concentration of substance in groundwater

No input required,values taken from previous worksheets

Summary of compliance data, attenuation and dilution factors

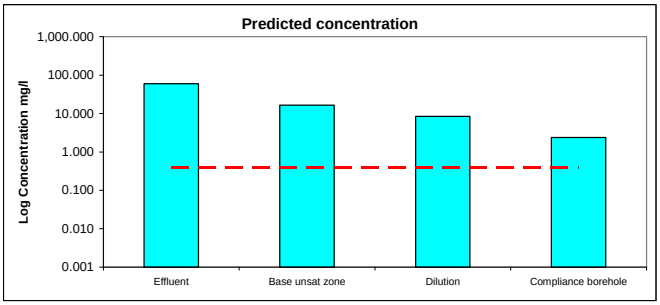
Substance		**Ammonium**		
Effluent concentration	C_e	6.00E+01	mg/l	
Compliance value or environmental standard	C_T	0.39	mg/l	
Distance to compliance point		50.00	m	
Attenuation factor - unsat zone	AFu	3.65E+00		
Dilution Factor	DF	1.95E+00		
Attenuation factor- sat zone	AFs	3.54E+00		

Predicted concentrations at compliance point

Concentration at base of unsaturated zone	C_{wt}	1.64E+01	mg/l	Attenuation in unsaturated zone only
Concentration in groundwater below drainage field	C_{gw}	8.41E+00	mg/l	Dilution taken into account
Concentration in groundwater at compliance point	C_{dcp}	2.38E+00	mg/l	Attenuation in saturated zone taken into account

Provisional discharge limit values

Based on attenuation in unsaturated zone	DL_1	1.43E+00	mg/l
Based on attenuation in unsaturated zone and dilution	DL_2	2.78E+00	mg/l
Based on dilution and attenuation in unsaturated and saturated zone	DL_3	9.84E+00	mg/l



4.0 Additional worksheets

4.1 Hydrogeological Calculations worksheet

In addition to the infiltration worksheets, a separate worksheet titled **hydrogeological calculations** is included (Figure 4.1). This worksheet is included to allow you to undertake a range of standard calculations that are frequently used by hydrogeologists.

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

Table 4.1 Hydrogeological calculations. These are independent of the worksheet calculations.

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

Figure 4.1 Hydrogeological calculations worksheet.

Simple hydrogeological calculations

These calculations are provided to allow additional hydrogeological calculations to be undertaken if required)

Parameter	symbol		unit	justification
Hydraulic conductivity	K	1.00E+01	m/d	
Hydraulic gradient	i	1.00E-02	unitless	
Effective porosity of aquifer	n	1.00E-01	fraction	
Thickness of saturated aquifer	b	5.00E+01	m	
Width of aquifer perpendicular to flow	w	5.00E+01	m	
Distance to receptor	x	1.00E+02	m	
Bulk density of aquifer materials	\	1.80E+00	g/cm^3	
Soil-water partition co-efficient	Kd	1.00E+00	l/kg	
Retardation factor of pollutant	R	19		

Groundwater flow velocity	v(GW)	1.16E-05	m/s	1.00E+00	m/day	3.65E+02	m/year
Time for groundwater to reach receptor	t(GW)	8.64E+06	seconds	1.00E+02	days	2.74E-01	years
Rate of groundwater flow through aquifer	Q	2.89E-03	m^3/s	2.50E+02	m^3/day	9.13E+04	m^3/year
Contaminant flow velocity	v(contam)	6.09E-07	m/s	5.26E-02	m/day	1.92E+01	m/year
Time for contaminant to reach receptor	t(contam)	1.64E+08	seconds	1.90E+03	days	5.21E+00	years

4.2 Ammonium Conversion worksheet

This Ammonium Conversion worksheet allows you to convert between different laboratory analyses of ammonium.

The ammonium ion (NH_4) is typically the dominant ion at neutral pH. However, in more alkaline water the ammonia (NH_3) ion becomes increasingly dominant.

Laboratories may report the analysis for ammonium as (NH_4) or as N (NH_4-N). In some cases the laboratory may have reported the result as Total ammonia (as NH_3) or as Total ammonia as N. Total ammonia is likely to include ammonium (NH_4) and ammonia (NH_3). In this case NH_4 may be converted to NH_3.

4.3 Porosity Calculator worksheet

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 (Box 4.1) are suitable for inclusion within the Attenuation in the Unsaturated Zone worksheets but not the effective porosity as used in the Attenuation in the Saturated Zone worksheet..

Box 4.1 Standard Equations for Porosity Calculator worksheet

The water filled porosity is calculated from:

$$\theta w = (\theta T) - (\theta a) \quad \text{(Equation 1)}$$

where:

$$\theta T = 1 - \frac{\rho}{d} \quad \text{(Equation 2)}$$

$$Vr = \frac{d}{\rho} - 1 \quad \text{(Equation 3)}$$

$$\theta a = \frac{(100 - S) * \theta T}{100} \quad \text{(Equation 4)}$$

$$S = \frac{MC * d}{Vr} \quad \text{(Equation 5)}$$

where:

θ_w = water filled porosity (fraction)

θ_a = air filled porosity (fraction)

θ_T = total porosity (fraction)

p = dry bulk density of unsaturated zone (g/cm^3)

d = particle density (g/cm^3)

MC = moisture content (% weight)

S = initial saturation (%)

Vr = void ratio (fraction)

It is important to note that these equations cannot be used to calculate the effective porosities used for the saturated zone attenuation assessment worksheet.

5.0 Degradation

The rate of degradation used for the unsaturated and saturated zone is likely to have a significant influence on calculated concentrations in groundwater and calculated discharge limit values. Guidance on the selection of degradation rates is given in Environment Agency (2011b) and additional information on transformation rates for ammonium is given in Environment Agency (2003).

Contaminant decay is modelled as a first order reaction and degradation is defined by a half-life expressed in days. 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 you use must relate to the behaviour of the chemical under similar environmental conditions (for example, redox, pH, contaminant concentrations, temperature, 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). If you are assessing contaminants that are not subject to degradation, such as heavy metals (non-radioisotopes) and chloride, or there is no evidence of degradation from field data, you should select the 'No degradation occurs' option.

For preference, you should obtain the degradation rates from studies which give a degradation rates that apply to both water and soil. If you have derived degradation rates from laboratory experiments based on water as the only phase this will overestimate the rate of degradation in groundwater, in which case you should select either the option 'No degradation occurs' or 'Degradation occurs in the dissolved phase only'.

6.0 Sensitivity analysis

The worksheets use a deterministic approach in the calculation of contaminant concentration and discharge limit values; they assign a single value for each parameter, which implies a high degree of confidence in that value. In practice, there will be uncertainty. We therefore recommend that you undertake a sensitivity analysis 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.

By varying selected input parameters in turn and observing the effect on the calculated concentrations, you can determine which parameters have the greatest effect on the results. If you then consider the likely range of values that apply to those parameters you can assess whether more data is needed to reduce uncertainty in the final result. The alternative is to adopt conservative values for the sensitive parameters and accept that this may result in higher calculated discharge limit values. Whichever approach is taken you should ensure that your assumptions are sufficiently protective of the environment.

Another common means of taking account of parameter variability 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, 2004) is used.

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

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