CoronaScreen

A Spreadsheet Tool for the Prediction of Contaminant Plume Length in Groundwater

Version 1.0

Analytical Model

User Guide

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Contents

1. Concept and model development

1.1 Introduction

This section describes the conceptual basis for the Analytical Model (AM), its set-up and physical dimensions. The development of the model and its adaptation to calculate plume lengths is presented.

The AM presented in this user guide is based on a closed-form analytical solution to the advective-dispersive-reactive transport equation for estimating the maximum length of a plume of organic contaminants in groundwater. The model requires input data for contaminant concentrations, background groundwater chemistry, longitudinal dispersivity, transverse horizontal and transverse vertical dispersivity, groundwater velocity, and source geometry (width and thickness). Maximum plume length is predicted as the horizontal distance (along an assumed centreline) from the source zone (or from a monitoring well exhibiting the highest concentration of the contaminant of interest) to where the contaminant is completely consumed by degradation.

The biodegradation of organic compounds in a contaminant plume can be represented by two cases, which describe the general distribution of degradation processes occurring in the plume. These cases are based on the Corona concept defining the contribution of degradation processes in plume development and include:

1. Plumes where degradation occurs predominantly at the fringe of the plume and is controlled by dispersion of electron acceptors into and electron donors out of the plume;
2. Plumes where degradation occurs predominantly in the anaerobic core and is normally diffusion-controlled and depends on availability of sediment-bound electron donors in the aquifer matrix.

In general, the first case describes the development of plumes containing organic or inorganic compounds which are transformed by oxidation processes, that occur when the contaminant (electron donor) is oxidised by an oxidant (electron acceptor) provided through mixing (via dispersion) of the contaminant plume and uncontaminated groundwater at the plume fringe. Examples include the oxidation of many aromatic hydrocarbon compounds (e.g. BTEX and phenols) and ammonium (NH_4^+) in landfill leachate plumes. It is known (and acknowledged in this analysis) that oxidation processes may occur in the anaerobic core of the plume as well as at the plume fringe. However, studies show that where oxidation is the primary pathway for transformation of a contaminant, oxidation processes occurring at the plume fringe are primarily responsible for most degradation in a plume (Thornton et. al., 1998; 2001a,b).

The second case describes the development of plumes containing organic or inorganic compounds which are transformed by reduction processes, rather than oxidation. In this case, the contaminant functions as an electron acceptor and is reduced by an electron donor present in the plume. The electron donors required for this transformation may be a co-contaminant, degradation product, naturally occurring organic compound or inorganic compound in the aquifer. Examples include the reduction of halogenated hydrocarbons (e.g. TeCE, TeCA, TCE and TCA, amongst others).

The AM presented here focuses on **the first type of plume only** (typically organic contaminants degraded by oxidation processes). Transformation of contaminants by reduction processes in the anaerobic core of the plume is not considered in the model. The conceptual model and governing equations behind the application of the AM for the performance assessment of attenuation in oxidising plumes are described below.

1.2 Governing assumptions and reactions

The model is based on the assumption that an oxidisable (typically organic) contaminant will be biodegraded, depending on availability of electron acceptors needed for degradation. Under the assumption that biodegradation occurs instantaneously and thus taking into account only the concentrations of electron donors (the contaminant) and electron acceptors (oxidants), the degradation processes in a plume can be represented as series of simple redox reactions. These are presented in terms of the number of electrons donated or gained, according to the stoichiometry of each half reaction (see Table 1). The number and type of redox half reaction included in the AM are determined from the range of electron donors (contaminants) and electron acceptors (oxidants).

Redox half reactions for a typical range of electron acceptors and electron donors (using phenol compounds and total organic carbon, TOC, as an example) are shown in Table 1. The number of electrons transferred in each half reaction is illustrated for each electron donor (e.g. 28 donated by phenol) and electron acceptor (e.g. 4 accepted by dissolved oxygen).

Table 1. Example of redox half-reactions

Electron donating reactions: *Oxidation of organic fractions*

Phenol: $C_6H_6O + 11H_2O \rightarrow 6CO_2 + 28e^- + 28H^+$

Cresols: $C_7H_8O + 13H_2O \rightarrow 7CO_2 + 34e^- + 34H^+$

Xylenols: $C_8H_{10}O + 15H_2O \rightarrow 8CO_2 + 40e^- + 40H^+$

TOC: $CH_2O + H_2O \rightarrow CO_2 + 4e^- + 4H^+$

Electron accepting reactions: *Reduction of aqueous oxidants*

Dissolved oxygen: $O_2 + 4e^- + 4H^+ \rightarrow 2H_2O$

Dissolved nitrate (denitrification): $NO_3^- + 5e^- + 6H^+ \rightarrow 1/2\, N_2 + 3H_2O$

Dissolved sulphate: $SO_4^{2-} + 8e^- + 8H^+ \rightarrow S^{2-} + 4H_2O$

1.3 Dissolved concentrations of electron donors and electron acceptors

The magnitude of the electron donor and electron acceptor inputs in the AM is defined by the concentration of both contaminants and oxidants, based on groundwater quality data for the uncontaminated aquifer and plume (see Table 2). The AM automatically converts the concentration of dissolved species (electron donors and electron acceptors) into electron equivalents. The basis for this conversion is that biodegradation is represented as a redox reaction between electron donors and electron acceptors. When converted to electron equivalents the reactions have unit stoichiometry, since one electron equivalent is donated and one electron equivalent is accepted. A further advantage of considering concentration in electron equivalents is that multiple electron donors and acceptors can be easily summed (Thornton et. al., 2001a). For instance, benzene and toluene concentrations can be combined, and reacted with the sum of oxygen and nitrate concentrations. A worked example illustrating how the model converts concentration to electron equivalents is given in Table 2 below.

Table 2. Example conversion of concentration in mg/l to electron equivalents

	Units	Electron donor	Electron acceptor
		Phenol	Oxygen
Half-reaction		$C_6H_6O + 11H_2O \rightarrow 6CO_2 + 28e^- + 28H^+$	$O_2 + 4e^- + 4H^+ \rightarrow 2H_2O$
Molecular weight	(g/mol)	94	32
Example concentration	(mg/l)	20	8
Concentration in moles	(mmol/l)	0.212	0.25
Electron transfer in half reaction	-	28	4
Concentration in electron equivalents	me^-/l	$ED_{max} = 5.93$	$EA_{max} = 1$

1.4 Governing assumptions and equations

The model is a modification of the analytical solution for three dimensional solute transport produced by Domenico and Robbins (1985). The conditions are that there is a continuous, which is conceptualised as a vertical plane, homogeneous aquifer properties, one-dimensional groundwater flow, and dispersion in three-dimensions. A conceptual model is shown in Figure 1.

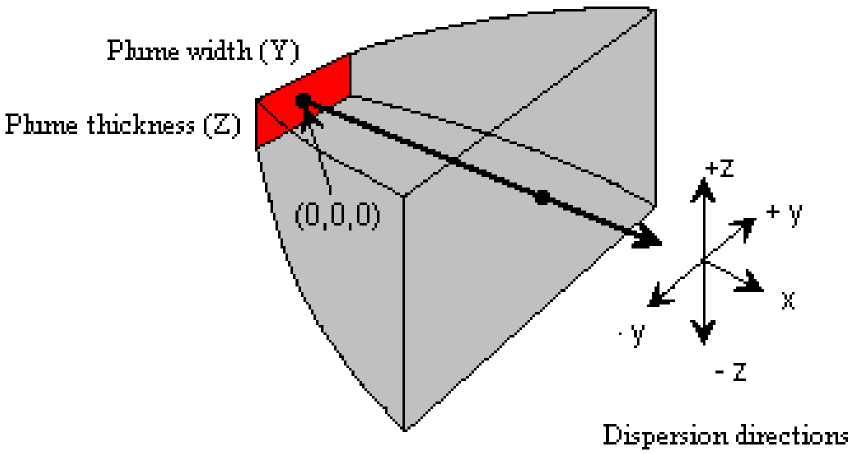


Figure 1. Schematics of the dispersion scenario considered in the analytical model

The governing equation for the analytical model is:

$$C_{ED} = \frac{C_{ED_{max}}}{8} \operatorname{erfc}\left(\frac{x - vt}{2\sqrt{\alpha_x vt}}\right)\left[\operatorname{erf}\left(\frac{y + \frac{Y}{2}}{2\sqrt{\alpha_y x}}\right) - \operatorname{erf}\left(\frac{y - \frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)\right]$$

$$\left[\operatorname{erf}\left(\frac{z + \frac{Z}{2}}{2\sqrt{\alpha_z x}}\right) - \operatorname{erf}\left(\frac{z - \frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)\right]\left(1 + \frac{C_{EA_{max}}}{C_{ED_{max}}}\right) - C_{EA_{max}} \qquad (1)$$

where C_{ED} is the concentration of the electron donor, v is the groundwater velocity, x, y and z are the coordinate axis with origin at the centre of the source, Y and Z are the width and thickness of the source area being modelled, t is the simulation time, C_{EDmax} is the source area electron donor concentration and C_{EAmax} is the background electron acceptors concentration.

1.5 Steady-state plume length

After a period of time a steady-state condition will be achieved for the plume when the continuous influx of contaminants from the plume source area is balanced by natural attenuation (primarily degradation) in the aquifer. Additionally, if a conservative estimate of the potential length of a contaminant plume is needed, the assumption of continuous contaminant input may be appropriate.

The plume length can be defined as the horizontal distance from the source area (or monitoring well) to where the value of the electron donor is completely consumed. The plume length can then be obtained by solving for “x” in Eq. (2) below:

$$\frac{C_{EA_{max}}}{C_{ED_{max}} + C_{EA_{max}}} = \left\{\operatorname{erf}\left[\frac{Y}{4(\alpha_y\, x)^{1/2}}\right]\operatorname{erf}\left[\frac{Z}{4(\alpha_z\, x)^{1/2}}\right]\right\} \qquad (2)$$

An exact solution to “x” can only be obtained through an iterative process. Thus, in the AM a search algorithm is adapted using the Excel built-in “Goal-seek” tool.

2. Application and scenario modelled

2.1 Introduction

This section presents the field scenario to which the AM can be applied. Data requirements and the design of monitoring wells to provide groundwater chemistry data for the AM simulation are described.

2.2 Monitoring well network for scenario modelled

The AM requires a minimum set of input parameters for simulations of contaminant plume evolution, as described in the previous chapter. This data and the anticipated analytical methods required to obtain it include:

- ☐ Aquifer physical and hydrogeological properties (e.g. hydraulic conductivity, hydraulic gradient, groundwater flow velocity, effective porosity) determined using relevant techniques (e.g. field-scale hydraulic tests and analysis of core samples from the aquifer, or appropriate literature values, where this is justified);
- ☐ Composition of background and plume groundwater chemistry, to provide concentrations of dissolved electron donors, electron acceptors, products of degradation processes and estimate solute concentration gradients across the plume fringe, using monitoring wells installed in uncontaminated locations, the plume source area and instrumented across the plume fringe.

This section focuses on the design of the monitoring well network to obtain the groundwater quality data required as input parameters for the AM simulations. The input parameters needed define the design and location of monitoring wells that must be installed at sites for the assessment using the AM. A monitoring network that fulfils these requirements is necessary for the model to correlate with the actual site under consideration. Figure 2 illustrates the typical location and instrumentation of monitoring wells for the typical or “standard” scenario that is assessed with the AM. The instrumentation of the individual monitoring wells required in this scenario is as follows:

- ☐ Upstream monitoring well

  This monitoring well provides concentration data for dissolved species (O_2, NO_3, SO_4) present in the background groundwater from the uncontaminated aquifer. A single screen monitoring well covering a section of the aquifer that samples a representative volume of uncontaminated groundwater is sufficient to provide this data (see section 3.3). If more than one single screened well exists, or if data from different depths at one or several locations from multilevel samplers are available, an averaged concentration can be used; see section 2.4 for a general discussion of this issue. Refer to section 3.3 for details of input parameters derived from this monitoring well. It is assumed in the model that the background concentrations of electron acceptors and other species in groundwater upstream of the plume source area are the same or very similar to concentrations found downstream above the plume (see below).

  Note that concentrations of TOC and contaminants should be measured in groundwater from this upstream monitoring well. In most aquifers and applications of the model the concentrations of TOC and contaminants found in the plume will be zero or close to zero in the background groundwater upstream of the site. However, there may be cases or aquifer settings where TOC is of interest or needs to be taken into account in the plume prediction, and a background TOC and/or contaminant concentration will be required for this (see section 3.3).

- ☐ Source area monitoring well

  This monitoring well is required to provide concentration data for all electron donor species present in contaminated groundwater from the plume source area. These species can include contaminants and other compounds which function as electron donors and which are biologically oxidised. A single screen well covering a representative part of the source area is the minimum installation required (see section 2.4 for discussion of integrating/using ranges of concentration).

If electron acceptors are part of the plume source term, they can be included, but must be given **negative** concentrations in the input file. Refer to section 3.5 for details of input parameters derived using data from this monitoring well.

- ❑ Downstream plume monitoring well
  This monitoring well is located in the plume downstream of the plume source area and is instrumented to sample uncontaminated and contaminated groundwater across the plume fringe. It is important that this monitoring well is instrumented as a **multilevel sampler** (MLS) with sufficient spatial resolution of sampling ports to characterise the vertical gradient of dissolved electron acceptors (O_2, NO_3, SO_4) across the plume fringe, measure electron donor (e.g. TOC and contaminant) concentrations in the plume and background groundwater and identify the "thickness" of the plume fringe mixing zone. Refer to sections 3.2, 3.3 and 3.6 for details of input parameters derived from this monitoring well. This monitoring well also provides data on the "background groundwater chemistry" and "plume source term composition" when the *alternative* monitoring well scenario is used to provide these inputs for the model (see section 2.3). It is assumed in the model that concentrations of dissolved electron acceptors measured in sample ports above the plume fringe are the same or very similar to those measured in the upstream monitoring well (see above).

On many sites, monitoring wells instrumented with a MLS capable of obtaining the necessary data for using the AM may not exist. In the planning stage of instrumenting a site to fulfill the data input requirements for the model, some depth-related solute concentration measurement is necessary to determine the approximate location of the plume fringe for placement of the downstream plume well. If existing monitoring wells do not indicate the location of the plume fringe, but exhibit contaminant concentrations that are representative of the plume, it is possible to instrument the MLS from the water table down to the depth indicated by the single screen plume monitoring wells. Obviously, the more defined the plume fringe area is from previous groundwater quality monitoring, the more resources can be saved because the MLS can be installed to sample specific depths across the plume fringe mixing zone. For placement of the upstream and the source area monitoring well, some estimate of the upstream edge of the plume is necessary from previous investigations.

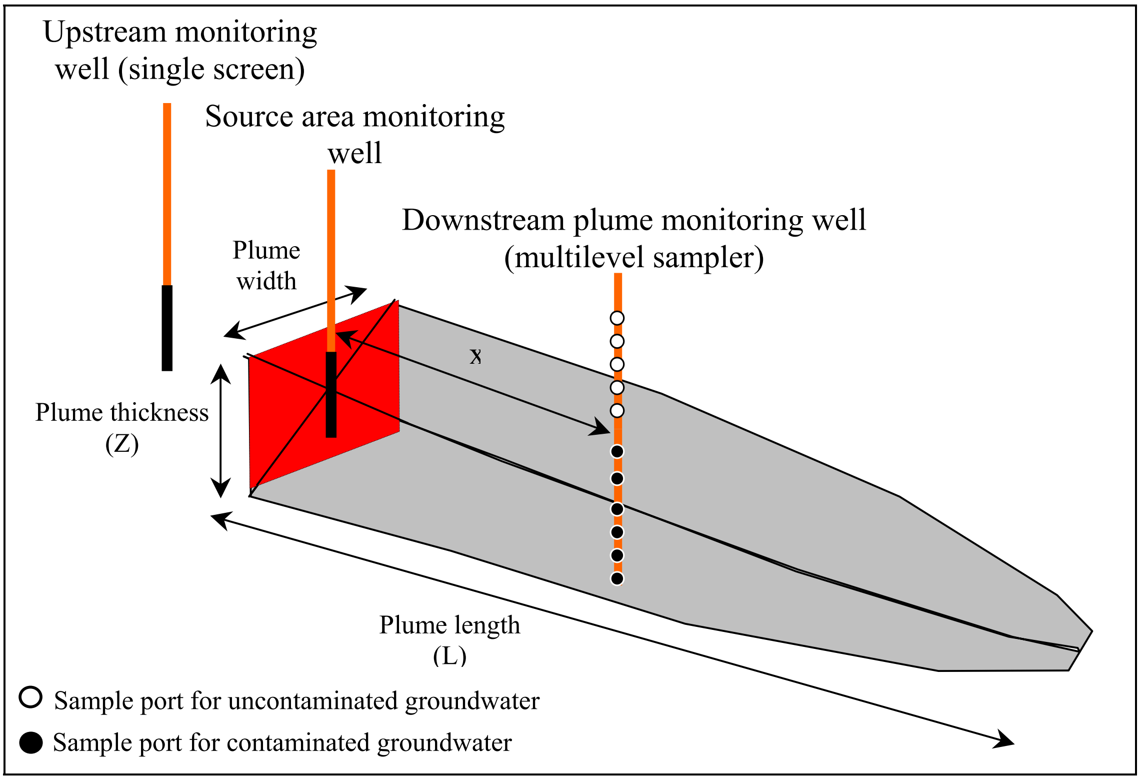


Figure 2. Schematic of monitoring well network for analysis of plume development using the AM

The “plume length” calculated by the AM for this monitoring well scenario equals the distance from the source area monitoring well to the downstream end of the plume. If the source area monitoring well is located a distance “s” downstream of the true plume source area, then this distance (“s”) is automatically added to the “plume length” predicted by the model to give a true plume length from the source area, given in the “Results” output section of the model.

2.3 Monitoring well network for alternative scenario

As a very stripped-down version, the ideal scenario described in the previous section can be modified to accommodate data from a very reduced “non-standard” monitoring network, using one MLS monitoring well only. In this *alternative* scenario, the downstream plume MLS monitoring well (as discussed in the previous section and shown in Figure 2) is also treated as the “source area” monitoring well by using the average contaminant concentrations measured inside the plume. These contaminant concentrations are obtained by sampling monitoring ports on the MLS which are located below the plume fringe. Furthermore, “background groundwater” concentrations of dissolved chemical species (measured in the upstream monitoring well) are assumed to be equal to the concentration above the plume measured in this MLS (this will generally be acceptable for most sites, but should be supported by relevant data). The “plume length” calculated by the AM for this monitoring well scenario equals the distance from the MLS monitoring well to the downstream end of the plume. This is the reference distance for the analysis, since the position of the MLS along the plume flow path is assumed to represent the location of the plume “source area” in this scenario. The distance along the plume flow path from the MLS to the true plume source area (“x” in Figure 2) would have to be added to the plume length calculated in this scenario, to yield an overall plume-length.

The “plume length” calculated by the AM for this monitoring well scenario equals the distance from the MLS monitoring well to the downstream end of the plume. This is the reference distance for the analysis, since the position of the MLS along the plume flow path is assumed to represent the location of the plume “source area” in this scenario. The distance along the plume flow path from the MLS to the true plume source area (“x” in Figure 2) is identical to the distance “s” from the source area to the source area monitoring well that is used in the standard monitoring well scenario. This distance is entered by the user and automatically added to the plume length calculated in this scenario, to yield an overall true plume length given in the “Results” output section of the model.

It should be noted that this alternative scenario does not account for any spatial variability in groundwater chemistry other than that which occurs across the plume fringe in the vertical direction. It therefore does not allow for averaging of concentrations and reconfirmation of values by measurements of groundwater chemistry at different locations across the site under consideration. Keeping in mind the heterogeneous nature of subsurface environments in general, the determination of inputs for the AM using this alternative monitoring well scenario has to be treated very carefully. The use of single data values to represent the whole site may increase the uncertainty in the results produced by the model.

2.4 Network of monitoring wells

The monitoring network introduced in section 2.2 includes the minimum number of monitoring wells to generate sufficient input data for the ideal monitoring well scenario. If additional monitoring wells in the same location of the plume (e.g. source area or downstream plume) exist or are planned, an average value can and should be used to reconfirm measurements for the dissolved concentrations of chemical species included in the AM. Also, sets of different parameter combinations within the range of measured values that occur across the site can be used to evaluate a variety of predicted plume lengths and contaminant spill scenarios (Thornton et. al., 2001a). Reliable estimates of plume width and depth need to be obtained for the AM. This may be achieved by the installation of additional monitoring wells at the upstream border of the source area, to delineate the plume depth and deduce the plume width in the transverse direction.

2.5 Summary of design options and data requirements for monitoring well networks

A summary of the data requirements and monitoring well design for the typical and alternative monitoring well scenarios is given below.

Monitoring Well Scenario	Monitoring Well Location	Monitoring Well Design	Parameters Measured	Comments
Typical (standard) case	Upstream	Single screen	O_2, NO_3, SO_4, TOC, and contaminants	❑ Background concentrations of species in uncontaminated aquifer
	Plume source area	Single screen	O_2, NO_3, SO_4, TOC, and contaminants	❑ Concentrations of species in contaminated aquifer
	Downstream plume	High-resolution MLS	O_2, NO_3, SO_4, TOC, and contaminants	❑ Profiles of solute concentrations are used to estimate thickness of plume fringe
Alternative case	Upstream Plume source area Downstream plume	High-resolution MLS	O_2, NO_3, SO_4, TOC, and contaminants	❑ "Background" concentrations of species are measured in uncontaminated groundwater above plume fringe ❑ "Source area" concentrations of species are measured in contaminated groundwater below plume fringe ❑ Profiles of solute concentrations are used to estimate thickness of plume fringe

3. Model parameters and data inputs

3.1 Introduction

The input parameters for the analytical model are entered in the spreadsheet marked "DataInput". Data are included in this spreadsheet under different categories of information, which provide the input terms for the equations used in the AM for the plume. These categories of information include parameter values related the following inputs:

- ☐ Plume source term
- ☐ Background groundwater chemistry
- ☐ Aquifer properties and hydrogeology
- ☐ Plume dimensions
- ☐ Plume fringe parameters

These inputs and the relevant parameters required for the calculation of each input in model simulations are explained below.

3.2 Plume source term composition

This data block includes concentrations (mg/l) of all species present in the source area, which function as an electron donor. These include dissolved oxidisable organic and inorganic contaminants and other compounds that define the chemical composition of the plume source term. It should be noted that the plume source term can include organic and inorganic compounds, according to the specific situation being modelled. This data is used to calculate electron donor fluxes into the plume from the source area. The plume "source term"composition is characterised using a single screen monitoring well located in the plume source area or sample ports on a MLS below the plume fringe, when the *alternative* monitoring well scenario is used (see section 2.2). The origin and use by the model of input values included in this data block are described below.

3.2.1 Organic compounds

The organic compounds included in the input data block for the plume source term are those commonly found as relatively mobile constituents in plumes of petroleum hydrocarbons, phenols and other organic chemicals. Acetate is often present in plumes as a degradation product of petroleum hydrocarbons and phenols. TOC is included for situations in which contaminant concentrations are represented by this parameter, or where the migration of this species is of primary interest in defining the plume length (e.g. landfill leachate plumes).

3.2.2 Inorganic compounds

Ammonium is included as an inorganic electron donor in the input data block for the plume source term. This species is commonly found as a contaminant in leachate plumes from landfills and plumes from coal carbonisation, gasworks or other similar facilities.

The model uses *dissolved* concentrations of electron donors to define the source term. Non-aqueous phase liquids (NAPLs) are not considered. Concentrations of dissolved electron donors representing the plume source term should be obtained from a monitoring well located below or immediately downgradient of the source area. It should be the same monitoring well that is used to define the plume depth or thickness.

3.2.3 Including electron acceptors in the source term

Electron acceptors, such as sulphate or nitrate, can be included in the source term input if the groundwater chemistry data from the source area monitoring well suggests that these species are components of the contaminant matrix (e.g. Thornton et. al., 2001a,b). This can be achieved by adding the new compound to the database and the list of contaminants included in the calculation (consult the user manual for a description of these actions). Since these (electron acceptor) compounds are part of the contaminant input block, they then need to be assigned a **negative** concentration to account for the fact that they are electron acceptors and not electron donors. This means it assumed in the model that electron acceptors and electron donors react upon entrance into the plume, so that the source term input of electron donors entering the plume is reduced.

3.3 Background groundwater chemistry

This data block includes input values which provide the chemistry of the background groundwater upgradient of the plume. The origin and use by the model of input values included in this data block are described below.

3.3.1 Background dissolved oxygen, nitrate and sulphate

A value of the dissolved O_2, NO_3 and SO_4 concentration (mg/l) in background groundwater is required to estimate the electron acceptors available as dissolved species. The concentration of dissolved O_2, NO_3 and SO_4 in the background groundwater can be obtained from a monitoring well located upgradient of the plume source area or those sampling ports of a multilevel sampler which are located above the plume fringe. It is assumed that these concentrations will be the same as the maximum values in background groundwater upstream from the source. However, the user has the option of inputting different values if data are obtained from different monitoring wells and / or there are spatial variations in background dissolved concentrations of these electron acceptors in the aquifer. **User-specified concentrations of dissolved O_2, NO_3 and SO_4 entered into this data block should be higher than those entered in the "plume residuals" data block, so that fluxes of dissolved electron acceptors entering the plume by dispersion can be calculated by the model.** A "pop-up" window is automatically activated to remind the user of this condition, should background values of dissolved O_2, NO_3 and SO_4 be less than the plume residual value.

3.3.2 Background dissolved total organic carbon

A value of the dissolved total organic carbon (TOC) concentration (mg/l) in background groundwater is required to estimate the concentration of TOC entering the plume from the source area. This is necessary when contaminant concentrations are measured or expressed in terms of TOC, rather than individual compounds or species. Conceptually, a TOC plume is the same as a plume of individual contaminants, with respect to consumption of electron acceptors during degradation reactions, and is treated as such in the model. In some cases, for example landfill leachate plumes, the migration of the TOC plume will control the attenuation of organic micropollutants which may be present in the leachate plume (Christensen et. al., 1994). Alternatively, there may be cases where the assessment of plume behaviour is required in a naturally anaerobic aquifer containing a high (or significant) background TOC concentration. The TOC arising from the plume source area must be corrected for this background TOC input from the aquifer in the model simulation.

3.3.3 Background contaminant concentration

In most cases, contaminants present in the plume will not be present in the background groundwater sampled in the upstream monitoring well. However, in cases where the target contaminants are also present in the upstream monitoring well (e.g. due to natural conditions or an unrelated contamination event), the concentration of these should be subtracted from the concentration measured in the source area monitoring well, and a net contaminant concentration entered in the input section for the plume source term composition.

3.4 Aquifer properties and hydrogeology

This data block includes input values for basic physico-chemical properties and hydrogeological parameters of the aquifer. The origin and use by the model of input values included in this data block are described below.

3.4.1 Groundwater flow velocity

A value of groundwater flow velocity, v (m/day), is input into the model in either of two ways. Groundwater velocity can be estimated from Darcy's Law using values of mean aquifer hydraulic conductivity (K), effective porosity (n_e) and hydraulic gradient (i), according to the following relationship:

$$v = \frac{K.i.}{n_e} \tag{3}$$

An estimate of groundwater velocity determined in this way requires separate estimation of aquifer hydraulic conductivity, effective porosity and hydraulic gradient from the site investigation undertaken for the plume analysis. Alternatively, an estimate of groundwater velocity can be input directly into the data block, if this is known from the site investigation, or if the other input terms (K, i, n_e) are unknown. The user has the option of selecting which method is used to input a value for groundwater velocity, by clicking the button marked "Restore velocity-equation". If this button is selected, groundwater velocity will be calculated by Darcy's Law using the appropriate input values, which will then be required in this data block.

3.4.2 Hydraulic conductivity

A value of hydraulic conductivity, K (m/day), is required to estimate groundwater velocity using Darcy's Law, when this method of input is selected. A site-specific value of K should be used for this input, as determined by appropriate hydraulic testing or other method of estimation.

3.4.3 Hydraulic gradient

A value of hydraulic conductivity, i (m/m), is required to estimate groundwater velocity using Darcy's Law, when this method of input is selected. A site-specific value of i should be used for this input, as determined by appropriate methods, such as measurement of groundwater elevation in monitoring wells. The plume ideally should be included in the network of monitoring wells used for this purpose.

3.4.4 Effective porosity

Effective porosity is defined as that proportion of saturated pore space in a unit volume of aquifer that contributes to fluid flow, which will be less than the total porosity. A value of effective porosity, n_e (dimensionless), is required to estimate groundwater velocity using Darcy's Law, when this method of input is selected. A site-specific value of n_e should be used for this input, as determined by appropriate methods, such as analysis of aquifer sediment or rock cores.

3.5 Plume source dimensions

This data block includes input values, which describe the geometry of the plume. The origin and use by the model of input values included in this data block are described below.

3.5.1 Plume width

A value of the plume width (m) is used to estimate the contaminant flux into the plume from the source area, which is conceptualised as a vertical plane perpendicular to the groundwater flow (see Figure 2). The plume width can be represented by the known or assumed width of the source area. Alternatively, plume width may be estimated using groundwater quality data from a transect of monitoring wells located across the groundwater flow direction, immediately downgradient of the source area.

3.5.2 Plume thickness

A value of the plume thickness (m) is used to estimate the contaminant flux into the plume from the source area, which is conceptualised as a vertical plane perpendicular to the groundwater flow (see Figure 2). The plume thickness can be represented by the known or assumed depth of the source area below the water table. For the scenario included in the model, this thickness should be taken as the maximum thickness of dissolved contaminants identified in a monitoring well located vertically below or immediately downgradient of the plume source area.

3.5.3 Distance: source to "source well"

The distance, "s" (m), from the plume source area to the downgradient location of the monitoring well used to provide the plume source term chemical composition ("source area monitoring well" in Figure 2) is required in this input. If the source area monitoring well is located within the true plume source area, this distance will be zero and is entered as such in this cell. This is the case for the typical (standard) monitoring well scenario shown in Figure 2. However, there may be practical reasons (e.g. access limitations) when the monitoring well used to determine the plume source term composition must be located some distance downstream of the source area (e.g underground storage tank). Since the plume length calculated by the AM is determined as the distance from the source area monitoring well, any offset distance of this monitoring well downstream of the true source area must be added to the plume length to give a "true" plume length from the "true" source area. The value of "s" entered by the user in this cell is automatically added to the plume length calculated from the location of the source area monitoring well to give a true plume length, as described.

When the *alternative* monitoring well scenario (see section 2.3) is used, the distance, s, entered by the user will be the distance from the true plume source area to the downstream MLS used to provide the composition of the plume source term. This distance will also equal the distance, x, entered for this MLS in the "Plume fringe parameters" input section (see section 3.6.1), when this monitoring scenario is used (see also Figure 2).

3.6 Plume fringe parameters

This input block includes values that determine the dispersive flux of solutes across the plume fringe. Due to the significance of the plume fringe with respect to overall degradation in the plume, the input parameters in this block are particularly important for the results of the AM.

It is not possible to enter more than one MLS at a time. If data from several MLS monitoring wells is available, these must be entered separately, and the results for every scenario compared, in order to identify the most realistic values for the site under consideration.

3.6.1 Distance: source to MLS well

The distance between the plume source and downstream monitoring well ("x" in Figure 2) is used to calculate the vertical transverse dispersivity, α_z, from the vertical plume fringe thickness, dz. The plume fringe thickness is not used directly as an input in the AM, but is instead used to indirectly estimate the vertical transverse dispersivity (see below). The plume fringe thickness, as defined by measurements from a MLS, will increase with distance from the plume source; thus, when calculating the dispersivity from the plume fringe thickness, the distance has to be taken into account. **A value of "x" greater than one must always be entered in this box to avoid "goal-seek error" or "#DIV/0!" messages occurring when the model is run.**

When the *alternative* monitoring well scenario (see section 2.3) is used, the distance, x, entered by the user in this input section will also be the same distance, s, entered for the distance from the source area to the source area monitoring well in the "Plume source dimensions" input section (section 3.5.3). This is because for this alternative monitoring scenario, a single MLS borehole, located downgradient of the plume source area, is simultaneously used to provide data on the background groundwater chemistry, plume fringe thickness and plume source term composition (see section 2.3).

3.6.2 Vertical fringe thickness

A value of the vertical thickness (m) of the "mixing zone" at the plume fringe is required to estimate the vertical transverse flux of dissolved electron acceptors in background groundwater into the plume by dispersion at the plume fringe. The "mixing zone" refers to the interval across the plume fringe where significant gradients in the spatial distribution of dissolved electron acceptors and electron donors exist, due to mixing by dispersion, of uncontaminated groundwater with contaminated groundwater in the plume. An estimate of the plume fringe thickness can be obtained from a profile of dissolved O_2, NO_3 and SO_4 versus depth, using a MLS instrumented across the plume fringe. The fringe thickness will be given by the vertical distance between the maximum and minimum concentration of these electron acceptors in the background groundwater and plume, respectively, as measured in the MLS profile instrumented across the plume fringe (see above). An alternative possibility is to calculate the vertical thickness of the plume fringe from an estimate of alpha z (see below) by clicking the button "Calc. dz from alpha_z". CoronaScreen uses the plume fringe thickness to estimate the vertical transverse dispersivity, alpha z, when this option is selected instead of inputting a value of alpha z directly in the AM (see section 3.6.3).

3.6.3 Vertical transverse dispersivity

Vertical transverse dispersivity, alpha z (m), can be either entered directly in the relevant cell of this input block (click the button "Calc. dz from alpha_z" in the right column if the cell is locked), or calculated indirectly from the vertical plume fringe thickness (click the button "Calc. alpha_z from dz" to calculate). When entering values directly, an estimate of alpha z (more commonly denoted α_z) may be obtained from the literature, where caution is advised in the selection of specific values, to ensure these are appropriate for the aquifer setting and properties assessed in the AM. **It is strongly recommended that alpha z is estimated for individual sites using a measurement of the plume fringe thickness obtained from a MLS installed across the plume fringe and the "Calc. alpha_z from dz" option in the model. Entering separate values of alpha z and/or the plume fringe thickness by decoupling the relationship which predicts these parameters (completed by accessing the "Dispersivity" tab in the "Calculation settings" section of the model) should only be undertaken by experienced modellers, using realistic values of these parameters for the scenario being evaluated with CoronaScreen.**

The link between user-defined inputs and the value of vertical dispersivity (alpha z, α_z) or plume fringe mixing zone thickness (dz) estimated in the CoronaScreen model is shown in Table 3. The table shows the data inputs that are required and the model outputs which are estimated when the relationship between alpha z and dz is either coupled or decoupled, as described above.

Table 3. Data inputs and model outputs for coupled and uncoupled link between vertical dispersivity and plume fringe mixing zone

Option Coupled	**Required data inputs**	**Model outputs[1]**	**Comments**
"Calc alpha z from dz"	☐ Distance: source to MLS well, "x" ☐ Vertical fringe thickness, "dz"	☐ Vertical dispersivity, "α_z"	☐ A value of "dz" is obtained from vertical profiles of electron acceptor concentrations across the plume fringe, using an MLS ☐ If "x" is changed for a fixed user-defined value of "dz", then "α_z" will change ☐ If "dz" is changed for a fixed user-defined value of "x", then "α_z" will change
"Calc dz from alpha z"	☐ Distance: source to MLS well, "x" ☐ Vertical dispersivity, "α_z"	☐ Vertical fringe thickness, "dz"	☐ A value of "α_z" is obtained from the literature[2] ☐ If "x" is changed for a fixed user-defined value of "α_z", then "dz" will change ☐ If "α_z" is changed for a fixed user-defined value of "x", then "dz" will change
Option Decoupled	☐ Vertical fringe thickness, "dz" ☐ Vertical dispersivity, "α_z"	☐ As entered by the user	☐ The distance from the source to the MLS has no effect on these model outputs ☐ Values of "dz" or "α_z" are not predicted by the model as the relationship between these is decoupled by the user

Notes

1. Model outputs in this case are either vertical dispersivity, "α_z", or vertical fringe thickness, "dz"
2. Values of "α_z" selected from the literature should be representative of the aquifer setting and scenario modelled

3.6.4 Horizontal transverse dispersivity

The value of horizontal transverse dispersivity, alpha y (m), cannot be entered directly, but is linked to alpha z by the following relation:

$$\alpha_y = \frac{\alpha_z}{DR_{z/y}} \tag{4}$$

where $DR_{z/y}$ denotes the ratio of alpha z over alpha y. This value is set to 0.1 by default, a value found in the literature to be typical for many contaminant plumes at field scale. However, if needed the user can change this ratio by clicking the button “Calculation settings…” and entering a new value on the “Dispersivity”-tab in the dialog shown.

4. Model outputs

4.1 Introduction

This section describes the outputs produced by the AM, which can be used to assess plume behaviour. The outputs are described under headings, which correspond directly with respective input data blocks in the "Analytical Model" spreadsheet, or are marked with the same colour to indicate relevant input data used to derive the outputs.

4.2 Plume length

The steady-state length of the plume is defined as the distance from the source area to the location along the plume flow path where the electron donor concentration equals zero. Calculations of plume length are shown under the section "Results". This value describes the length that the contaminant plume will reach when it achieves a steady-state condition. This is the length of a mixed plume of "lumped" electron donors, expressed as concentration of electron equivalents (see Chapter 1), which has been calculated from the sum of contaminants in the plume source term. Individual contaminant travel at the same velocity and are considered to be part of a homogeneous mixture of contaminants, as retardation due to sorption is not taken into account in the AM. The plume length given in the "Results" section is the true plume length from the site source area, taking into account the downgradient distance from the site of the monitoring well used to provide the plume source term composition for the different monitoring scenarios (see section 3.5 and 3.6).

4.3 Time to steady-state length

The time required for the plume to reach a steady-state length is displayed on the "AS_Output"-worksheet. As with plume length, this value represents the travel time for a mixture of contaminants, all expressed in electron equivalents. Individual contaminants are considered to travel at the same velocity. However, this value of time is not equal to the plume length divided by the groundwater flow velocity v; an analytical solution using longitudinal dispersivity, alpha x, has been applied to estimate this value. The calculation of this parameter can be switched off separately on the Analytical-tab under "Calculation settings…", in case the iteration to estimate this parameter causes problems.

4.4 Centreline profile

The concentration profile of electron donors (contaminant) in electron equivalents along the idealised plume centreline (horizontal distance) for a given simulation time is illustrated in Figure 3. The centreline output screen shows the concentration along the centreline of the plume with y = z = 0. All concentrations are displayed in units of e/l (electron equivalents / litre).

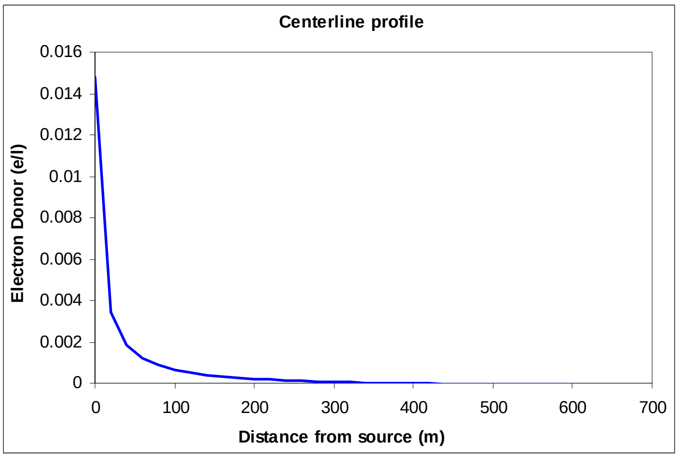
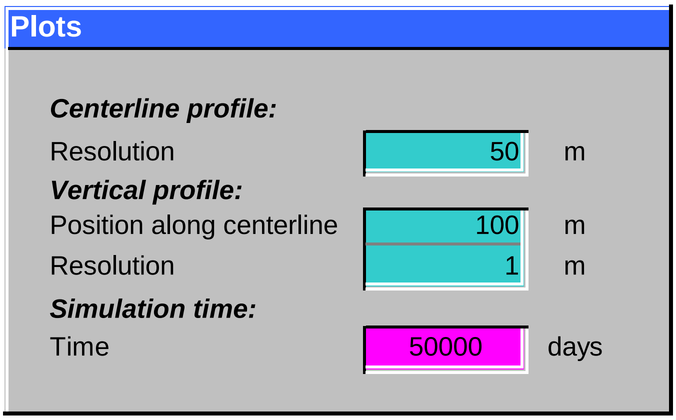


Figure 3. Example of a centreline profile for a contaminant plume, showing predicted concentration of electron donor (contaminant) as a function of distance along the plume flow path

It should be noted that the AM will generate this profile for an idealised centreline network of monitoring wells even if this network does not exist for the plume. Where such a monitoring network is present, this profile may be compared with the field data (which needs to be converted to the same units as the model output). In such cases, differences between actual and modelled contaminant concentrations may reflect limitations in the installation of a monitoring network along a presumed centreline for the plume.

If the predicted plume migration is greater than the scale of the plot, the resolution can be re-adjusted in the uppermost cell of the section named “Plots” (Figure 4), to visualize the plume at a different scale.



Plots

Centerline profile:

Resolution 50 m

Vertical profile:

Position along centerline 100 m

Resolution 1 m

Simulation time:

Time 50000 days

Figure 4. Input box for adjustment of graphs when scaling outputs of predicted plume length

To obtain the steady state profile for the plume, a value larger than the time needed to reach steady-state has to be entered for the simulation time.

4.5 Vertical profile

The vertical profile shows the predicted distribution of reactive solutes across the plume fringe as a function of depth, where electron acceptors (EA) and electron donors (ED) are mixed and reacted into and out of the plume, respectively. The concentration units are electron equivalents / litre.

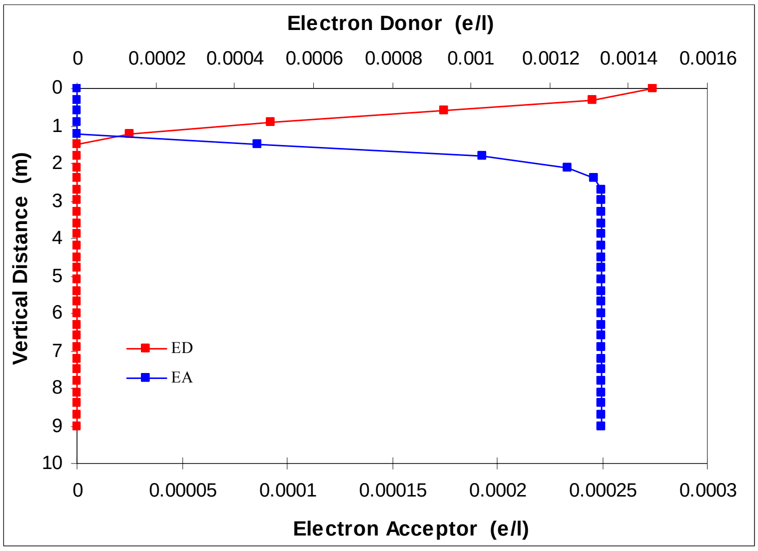


Figure 5. Example of a predicted vertical profile of electron donors and electron acceptors across the plume fringe, illustrating the solute gradients and mixing zone

The vertical profile can be adjusted with regard to the resolution and position along the centreline. For example, if profiles at various points downgradient from the source area are of interest, this position can be entered in the two central cells of the “Plots” section (Figure 4). As with the centreline profile, a large value for simulation time must be entered to view a steady state profile.

5. References

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Thornton, S.F., Davison, R.M., Lerner, D.N. & Banwart, S.A. (1998). Electron balances in field studies of intrinsic bioremediation. In : GQ98: *Groundwater quality: Remediation and Protection*, Tübingen, Germany, Sept 1998. IAHS Publ. No. 250, 273-282.

Thornton, S.F., Lerner, D.N. & Banwart, S.A. (2001a). Assessing the natural attenuation of organic contaminants in aquifers using plume-scale electron and carbon balances: model development with analysis of uncertainty and parameter sensitivity. *J. of Contaminant Hydrology*, 53, 199-232.

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