USER'S GUIDE

Prediction of Groundwater Quality Improvement Down-Gradient of In Situ Permeable Treatment Barriers and Fully Remediated Source Zones

ESTCP Project ER-0320

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DGCHANGE V1.0 USER'S GUIDE

A tool for estimating dissolved contaminant concentration reductions with time in near-field monitoring wells down-gradient of permeable treatment barriers (PTBs).

1.0 OVERVIEW

DGCHANGE v1.0 estimates dissolved contaminant concentration reductions with time in near-field monitoring wells down-gradient of permeable treatment barriers (PTBs). In this spreadsheet-based tool the aquifer is represented as a series of horizontal layers and the user enters layer-specific aquifer characteristics. The output is presented graphically in three main formats: a) a cross-section snapshot of dissolved concentrations along the groundwater flow path at some user-specified time, b) a table of dissolved concentrations vs. time in each layer at some user-defined down-gradient location, and c) as a plot of expected monitoring well dissolved concentration vs. time at some user-defined down-gradient location for layer thickness- and layer discharge-weighted averages.

The underlying fundamental basis and governing equations upon which DGCHANGE v1.0 is based are described in Appendix A. This appendix provides a step-by-step user's guide for DGCHANGE v1.0 and is organized by each of the tool's four worksheets that focus on model inputs, a cross-section snapshot, and changes with time at a monitoring well.

DGCHANGE v1.0 was developed as part of ESTCP Project ER-0320 "*Prediction of Groundwater Quality Down-Gradient of In Situ Permeable Treatment Barriers and Fully-Remediated Source Zones*", and its application is illustrated in the final report for that project found at www.estcp.org.

2.0 DGCHANGE v1.0 INPUTS

The "**inputs**" worksheet is the first worksheet found in DGCHANGE v1.0, and the values input here are utilized in other worksheets. The **inputs** worksheet is color-coded, and the user may enter items into the yellow cells only; all other cells include either text or calculated values. The following steps should be taken as the user enters inputs into the inputs worksheet (see Figure UG-1).

- Save the DGCHANGE v1.0 file with a new name (i.e. use the site name) so that you can easily reuse the original file.
- Enter the total thickness of the water-saturated interval of interest into column E, row 4.
- Enter the depth below ground surface (BGS) to the top of the water-saturated interval of interest into column E, row 5.
- Enter the distance down-gradient of interest from the permeable reactive barrier (PRB) into column E, row 6.
- Enter the chemical name of interest into column E, row 7.
- Enter the organic carbon sorption coefficient (K_{oc}) for the chemical of interest into column E, row 8. There are internet –accessible sources of information for this property (e.g., http://www.epa.gov/superfund/resources/soil/attachc.pdf)

- DGCHANGE v1.0 automatically divides the total thickness into ten evenly-spaced vertical intervals, if desired; you can over-ride these interval thicknesses by entering user-specified thicknesses into columns A and C, rows 13 thru 23.
- Enter qualitative descriptions of materials found in each interval into column D, rows 13 thru 23.
- Enter the hydraulic conductivity K for each layer in units of [cm/s] into column E, rows 13 thru 23. These values should derive from field data and should be consistent with the qualitative descriptions entered in Step 8.
- Enter the initial (time = 0) dissolved concentration C for each layer in units of [μg/l] into column F, rows 13 thru 23. These values should derive from field data.
- Enter the water-filled porosity ϕ for each layer in units of [vol-H2O/vol-soil] into column G, rows 13 thru 23. Typical values for granular materials are in the range 0.25 – 0.45 cm^3-H_2O/cm^3-soil.
- Enter the hydraulic gradient (dh/dx) for each layer in units of [cm/cm = m/m = ft/ft] into column I, rows 13 thru 23. Typically, the same value will be entered for each layer.
- Enter the soil bulk density ρ_b for each layer in units of [g-soil/cm^3] into column J, rows 13 thru 23. In the absence if site-specific data, a value of 1.7 g-soil/cm^3 is a reasonable estimate.
- Enter the fraction of organic carbon in soil f_{oc} for each layer in units of [g-OC/g-soil] into column K, rows 13 thru 23. Typical values for most granular materials fall in the range 0.005 – 0.02 g-OC/g-soil. Some feel that values less than 0.005 g-OC/g-soil will underestimate sorption, even if the f_{oc} value is less than 0.005 g-OC/g-soil.

Please note that all yellow cells must contain values for the tool to work correctly.

3.0 VERTICAL CROSS-SECTION SNAPSHOT VIEW

Once the **Inputs** worksheet contains data for all yellow colored cells, the "**Cross-Section Snapshot"** worksheet shown in Figure UG-2 may be used.

To use this worksheet, enter the time (in units of days) for which a cross-section snapshot is desired into column G, row 2.

The resulting output is presented as a cross-section snapshot for the time entered, oriented along the direction of groundwater flow, and showing locations where clean water is expected to be found. The cross-section is displayed in columns F thru T, from rows 6 thru 16. This cross-section corresponds to a single time snapshot, as defined by the input in column G, row 2. Cells colored red indicate contaminated (non-treated) water (these cells are assigned the corresponding user-identified initial concentration). Cells colored light blue indicate clean water (water treated by the PRB; these cells are assigned a concentration of 0 μg/l).

Rows 17 and 18 indicate corresponding thickness-weighted average concentrations (Equation UG.1 below) and layer discharge-weighted average concentrations (Equation UG.2 below) at different distances down-gradient of the PTB. Equation UG.2 assumes that the horizontal hydraulic gradient is the same in each layer i.

$$\{C\} = \frac{\sum_i C_i H_i}{\sum_i H_i} \text{ (layer thickness-weighted average)} \qquad \text{(UG.1)}$$

$$\{C\} = \frac{\sum_i C_i K_i H_i}{\sum_i K_i H_i} \text{ (layer discharge-weighted average)} \qquad \text{(UG.2)}$$

4.0 ESTIMATED DISSOLVED CONCENTRATION CHANGES WITH TIME AT MONITORING WELLS

Using the values in the **Inputs** worksheet, the expected changes in concentrations in each layer with time at a fixed distance down-gradient are calculated in the **Changes with time at MW** worksheet shown in Figure UG-3.

To use this worksheet, enter the time interval (in units of days) for which concentration vs. time projections are desired into column G, row 1. Next, enter the distance down-gradient of the PTB (in units of feet) where the monitoring well is to be located.

The resulting output is a tabular summary of the time evolution of treated water and contaminant concentrations in each layer, from the depths indicated in columns A and C, and over the time periods (in days) indicated in row 4. The time evolution is displayed in columns F thru P, from rows 6 thru 16. As in the cross-section worksheet, cells colored red indicate untreated water (these cells are assigned the corresponding user-identified initial concentration). Cells colored light blue indicate PRB-treated water (these cells are assigned a concentration of 0 μg/l).

Rows 17 and 18 present the corresponding thickness-weighted average concentrations (equation UG.1) and layer discharge-weighted average concentrations (Equation UG.2) for samples collected from a well at this location.

5.0 CONCENTRATION VS. TIME PLOT

The results calculated in the **Changes with time at MW** worksheet are used to generate the **Concentration vs. Time Plot** worksheet, which presents interval thickness-weighted average and the interval flow-weighted average concentrations as shown in Figure UG-4.

Introduction: DGCHANGE V1.0 allows user to estimate dissolved contaminant concentration reductions with time in near-field down-gradient monitoring wells after installation of a permeable reactive barrier (PRB). The aquifer is represented as a series of horizontal layers and the user enters layer-specific aquifer characteristics into the spreadsheet (yellow cells). The output is presented graphically in three worksheets: a) a "cross-section snapshot" of dissolved concentrations along the groundwater flow path at some user-specified time, b) a "Changes with time at Monitoring Well" (MW) concentrations vs. time worksheet for each layer at some user-defined down-gradient location, and c) an expected monitoring well dissolved "Concentration vs. Time Plot" at some user-defined down-gradient location for layer thickness- and layer discharge-weighted averages.

All yellow-shaded cells are input cells, enter all inputs into the "inputs" worksheet first.

Total thickness of the water-saturated interval of interest	10	[ft]
Depth below ground surface (bgs) to top of water-saturated interval of interest	9	[ft]
Distance Down-Gradient of Interest from the PRB	300	[ft]
Chemical Name	MTBE	
Organic Carbon Sorption Coefficient (K_{oc}) for Chemical of Interest	20	[L-H_2O/kg-OC]

Discretization and Qualitative Description of Saturated Interval of Interest (note: the spreadsheet automatically divides the total thickness into 10 evenly-spaced intervals, but you can also over-ride this and enter different thicknesses to each layer)				**Estimated Physical Properties of Each Discrete Interval Identified Below**								**Calculations**	
Top of Layer [ft BGS]		Bottom of Layer [ft BGS]	Qualitative Description of Materials Found in this Interval (user-entered)	Hydraulic Conductivity [K] [cm/s]	Initial Concentration [C] [ug/L]	Water-Filled Porosity [ϕ] [vol-H_2O/ vol-soil]	Layer Thickness [H] (calculated) [ft]	Hydraulic Gradient [i] [ft/ft]	Soil Bulk Density [ρ_b] [g-soil/cm^3]	Fraction of Organic Carbon in Soil [f_{oc}] [g-OC/g-soil]	Solute Retardation Factor [R] (calculated) [unitless]	Average Linear Velocity in Each Interval [ft/d]	Flow per Unit Width of Each Interval [ft^3/ft-d]
9.0	to	10.0	silt and/or fine sands	1.0E-05	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.00	0.00
10.0	to	11.0	silt and/or fine sands	1.1E-02	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.41	0.41
11.0	to	12.0	fine sand	3.1E-03	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.12	0.12
12.0	to	13.0	fine sand	1.6E-03	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.06	0.06
13.0	to	14.0	fine sand	9.3E-03	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.35	0.35
14.0	to	15.0	heterogeneous mix of fine/coarse sands with intermittent gravels	6.3E-03	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.24	0.24
15.0	to	16.0	heterogeneous mix of fine/coarse sands with intermittent gravels	5.2E-03	7679.00	0.30	1.00	0.004	1.70	0.005	1.57	0.20	0.20
16.0	to	17.0	heterogeneous mix of fine/coarse sands with intermittent gravels	4.3E-02	6047.00	0.30	1.00	0.004	1.70	0.005	1.57	1.62	1.62
17.0	to	18.0	heterogeneous mix of fine/coarse sands with intermittent gravels	1.7E-02	6047.00	0.30	1.00	0.004	1.70	0.005	1.57	0.66	0.66
18.0	to	19.0	heterogeneous mix of fine/coarse sands with intermittent gravels	6.3E-03	6047.00	0.30	1.00	0.004	1.70	0.005	1.57	0.24	0.24
19.0	to	20.0	heterogeneous mix of fine/coarse sands with intermittent gravels	2.4E-02	6047.00	0.30	1.00	0.004	1.70	0.005	1.57	0.90	0.90

Figure UG-1. The **Inputs** worksheet from DGCHANGE v1.0. The sample inputs in the yellow-shaded cells represent data from the NBVC MTBE bio-barrier site discussed in Chapters 3 and 4 of the Final Report for ESTCP Project ER-0320 "*Prediction of Groundwater Quality Down-Gradient of In Situ Permeable Treatment Barriers and Fully-Remediated Source Zones*", found at www.estcp.org.

t =	1700	days	Concentrations Displayed in Cells at Each Distance and Depth

This information retrieved from the inputs worksheet					Distance Down-Gradient from PRB Treatment Zone-->														
Top of Layer [ft BGS]		Bottom of Layer [ft BGS]	Qualitative Description of Materials Found in this Interval (user-entered)	Distance Travelled in time t [ft]	0 [ft]	30 [ft]	60 [ft]	90 [ft]	120 [ft]	150 [ft]	180 [ft]	210 [ft]	240 [ft]	270 [ft]	300 [ft]	330 [ft]	360 [ft]	390 [ft]	420 [ft]
9.0	to	10.0	silt and/or fine sands	0.41	0	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679
10.0	to	11.0	silt and/or fine sands	442.93	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11.0	to	12.0	fine sand	125.50	0	0	0	0	0	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679
12.0	to	13.0	fine sand	63.57	0	0	0	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679
13.0	to	14.0	fine sand	383.05	0	0	0	0	0	0	0	0	0	0	0	0	0	7679	7679
14.0	to	15.0	heterogeneous mix of fine/coarse sands with intermittent gravels	257.14	0	0	0	0	0	0	0	0	0	7679	7679	7679	7679	7679	7679
15.0	to	16.0	heterogeneous mix of fine/coarse sands with intermittent gravels	212.44	0	0	0	0	0	0	0	0	7679	7679	7679	7679	7679	7679	7679
16.0	to	17.0	heterogeneous mix of fine/coarse sands with intermittent gravels	1759.41	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.0	to	18.0	heterogeneous mix of fine/coarse sands with intermittent gravels	713.61	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18.0	to	19.0	heterogeneous mix of fine/coarse sands with intermittent gravels	259.61	0	0	0	0	0	0	0	0	0	6047	6047	6047	6047	6047	6047
19.0	to	20.0	heterogeneous mix of fine/coarse sands with intermittent gravels	980.18															
Interval thickness-weighted average concentration [ug/L]					0	698	698	1396	1396	2094	2094	2094	2792	4040	4040	4040	4040	4738	4738
Interval flow-weighted average concentration [ug/L]					0	1	1	95	95	280	280	280	594	1276	1276	1276	1276	1842	1842

Figure UG-2. The **Cross-Section Snapshot** worksheet from DGCHANGE v1.0. Blue shaded areas represent distances and depths down-gradient where treated water is projected to have migrated to within the time entered at the top of this worksheet. Red areas represent zones still at their initial concentrations. Calculated interval thickness- and flow-weighted average concentrations are presented at the bottom of the table for each distance down-gradient. The sample inputs represent data from the NBVC MTBE bio-barrier site discussed in Chapters 3 and 4 of the Final Report for ESTCP Project ER-0320 "*Prediction of Groundwater Quality Down-Gradient of In Situ Permeable Treatment Barriers and Fully-Remediated Source Zones*", found at www.estcp.org.

				Time Window	1700	d									
				Distance	50	ft	Concentrations Displayed in Cells at Each Time and Depth								
This information retrieved from the inputs worksheet															
Top of Layer [ft BGS]		Bottom of Layer [ft BGS]	Qualitative Description of Materials Found in this Interval (user-entered)	Time to Travel This Distance [d]	0 [d]	170 [d]	340 [d]	510 [d]	680 [d]	850 [d]	1020 [d]	1190 [d]	1360 [d]	1530 [d]	1700 [d]
9.0	to	10.0	silt and/or fine sands	207256.94	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679	7679
10.0	to	11.0	silt and/or fine sands	191.90	7679	7679	0	0	0	0	0	0	0	0	0
11.0	to	12.0	fine sand	677.31	7679	7679	7679	7679	0	0	0	0	0	0	0
12.0	to	13.0	fine sand	1337.14	7679	7679	7679	7679	7679	7679	7679	7679	0	0	0
13.0	to	14.0	fine sand	221.90	7679	7679	0	0	0	0	0	0	0	0	0
14.0	to	15.0	heterogeneous mix of fine/coarse sands with intermittent gravels	330.55	7679	7679	0	0	0	0	0	0	0	0	0
15.0	to	16.0	heterogeneous mix of fine/coarse sands with intermittent gravels	400.11	7679	7679	7679	0	0	0	0	0	0	0	0
16.0	to	17.0	heterogeneous mix of fine/coarse sands with intermittent gravels	48.31	6047	0	0	0	0	0	0	0	0	0	0
17.0	to	18.0	heterogeneous mix of fine/coarse sands with intermittent gravels	119.11	6047	0	0	0	0	0	0	0	0	0	0
18.0	to	19.0	heterogeneous mix of fine/coarse sands with intermittent gravels	327.42	6047	6047	0	0	0	0	0	0	0	0	0
19.0	to	20.0	heterogeneous mix of fine/coarse sands with intermittent gravels	86.72	6047	0	0	0	0	0	0	0	0	0	0
Interval thickness-weighted average concentration [ug/L]					7086	5436	2792	2094	1396	1396	1396	1396	698	698	698
Interval flow-weighted average concentration [ug/L]					6513	2496	594	280	95	95	95	95	1	1	1

Figure UG-3. The **Changes with time at MW** worksheet from DGCHANGE v1.0. Blue shaded areas represent time and depth combinations for the appearance of treated water at a fixed monitoring well location down-gradient of the PTB. Red areas represent time and depth combinations still at their initial concentrations. Calculated interval thickness- and flow-weighted average concentrations are presented at the bottom of the table for each time given. The sample inputs represent data from the NBVC MTBE bio-barrier site discussed in Chapters 3 and 4 of the Final Report for ESTCP Project ER-0320 "*Prediction of Groundwater Quality Down-Gradient of In Situ Permeable Treatment Barriers and Fully-Remediated Source Zones*", found at www.estcp.org.

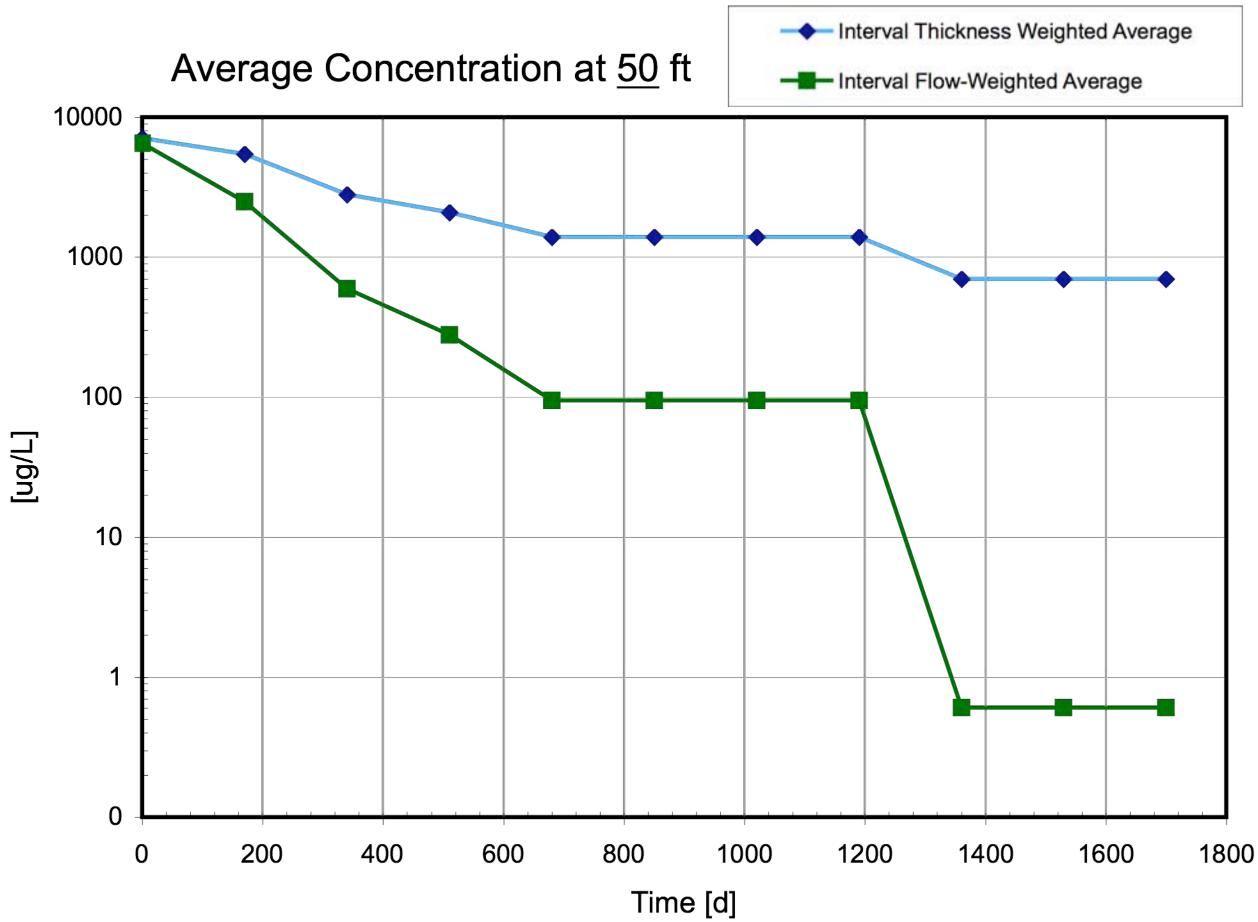

Figure UG-4. The **Concentration vs. Time Plot** generated from the results in the **Changes with time at MW** worksheet in DGCHANGE v1.0. Calculated interval thickness- and flow-weighted average concentrations are plotted here. The sample inputs represent data from the NBVC MTBE bio-barrier site discussed in Chapters 3 and 4 of the Final Report for ESTCP Project ER-0320 "*Prediction of Groundwater Quality Down-Gradient of In Situ Permeable Treatment Barriers and Fully-Remediated Source Zones*", found at www.estcp.org.

APPENDIX A

THEORETICAL BASIS FOR THE SPREADSHEET TOOL DGCHANGE v1.0

DGCHANGE v1.0 was developed using a simplified form of the General Transport Equation (Fetter 1999) for cases of layered one-dimensional advection-dominated scenarios. Advective transport is the process by which dissolved constituents travel with flowing groundwater, and advection-dominated scenarios are ones for which the effects of dispersion, diffusion, and reaction are much less-significant than the effects of advection. In the case of one-dimensional flow, groundwater movement in each layer i can be characterized by an average linear velocity as described by Equation A.1:

$$v_i = (K_i/\theta_{m,i})^* \, (dh/dx) \qquad \text{(A.1)}$$

where:

v_i	=	average linear velocity in layer i [cm/s]
K_i	=	horizontal hydraulic conductivity in layer i [cm/s]
$\theta_{m,i}$	=	water-filled effective porosity in layer i [cm^3-H_2O/cm^3-soil]
(dh/dx)	=	horizontal hydraulic gradient in the direction of flow (dh/dx is the same in all layers because the flow is one dimensional) [cm/s]

The change in dissolved groundwater concentration in each layer C_i [g/cm^3-H_2O] with down-gradient distance x [cm] and time t [s] is described by:

$$\frac{\partial C_i}{\partial t} = -\frac{v_i}{R_i}\frac{\partial C_i}{\partial x} \qquad \text{(A.2)}$$

where R_i is referred to as the retardation factor for layer i, and contains partitioning information:

$$R_i = 1 + \frac{H_c\,\theta_{v,i}}{\theta_{m,i}} + \frac{K_{s,i}\,\rho_{b,i}}{\theta_{m,i}} \qquad \text{(A.3)}$$

and:

H_c	=	Henry's Law Constant [(mg/cm^3-vapor)/(mg/cm^3-H_2O)]
$\theta_{v,i}$	=	vapor-filled porosity in layer i [cm^3-vapor/cm^3-soil]
$\theta_{m,i}$	=	water-filled porosity in layer i [cm^3-H_2O/cm^3-soil]
$K_{s,i}$	=	sorption coefficient to soil in layer i [(mg/g-soil)/(mg/cm^3-H_2O)] = $f_{oc}K_{oc}$

K_{oc} = sorption coefficient to organic carbon [(mg/g-OC)/(mg/cm^3-H_2O)]
$f_{oc,i}$ = fraction of organic carbon in soil in layer i [g-OC/g-soil]

For problems involving dissolved transport in aquifers, the first term on the right-hand-side of Equation (A.3) is typically negligible when $H_c < 0.1$ (mg/cm^3-vapor)/(mg/cm^3-H_2O).

For PTB problems, we can approximate the boundary condition and initial conditions as $C_i(x=0, t) = C_{treated}$ and $C_i(x, t=0) = C_i^o(x)$, and the solution to Equations (A.1) through (4.3) becomes:

$$C_i(x,t) = C_{treated,i} \text{ for } x \leq (K_i(dh/dx)t/\theta_i R_i)$$
$$C_i(x,t) = C_{io}(x - K_i(dh/dx)t/\theta_i R_i) \text{ for } x > (K_i(dh/dx)t/\theta_i R_i) \quad \text{(A.4)}$$

For PTB scenarios with $C_i(x=0, t) = 0$ (total treatment) and $C_i(x, t=0) = C^o$ (uniform initial conditions Equations (A.4) becomes:

$$C_i(x,t) = 0 \text{ for } x \leq (K_i(dh/dx)t/\theta_i R_i)$$
$$C_i(x,t) = C^o \text{ for } x > (K_i(dh/dx)t/\theta_i R_i) \quad \text{(A.5)}$$

Equations (A.4) and (A.5) apply to any horizontal plane with the x-axis aligned in the direction of groundwater flow.

Most groundwater samples are collected from monitoring wells screened over finite, but not small, intervals. For example, many groundwater monitoring well screen lengths are 3 – 5 m long. Thus, the sample represents a weighted average of groundwater entering the well at different depths spanned by the well screen. This weighted average likely represents something ranging from a layer thickness-weighted average to a layer discharge-weighted average as described in Equations (A.6) and (A.7), respectively:

$$\{C\} = \frac{\sum_i C_i H_i}{\sum_i H_i} \text{ (layer thickness-weighted average)} \quad \text{(A.6)}$$

$$\{C\} = \frac{\sum_i C_i K_i H_i}{\sum_i K_i H_i} \text{ (layer discharge-weighted average)} \quad \text{(4.7)}$$

where H_i = layer thickness [cm]

DGCHANGE v1.0 performs the calculations outlined above.