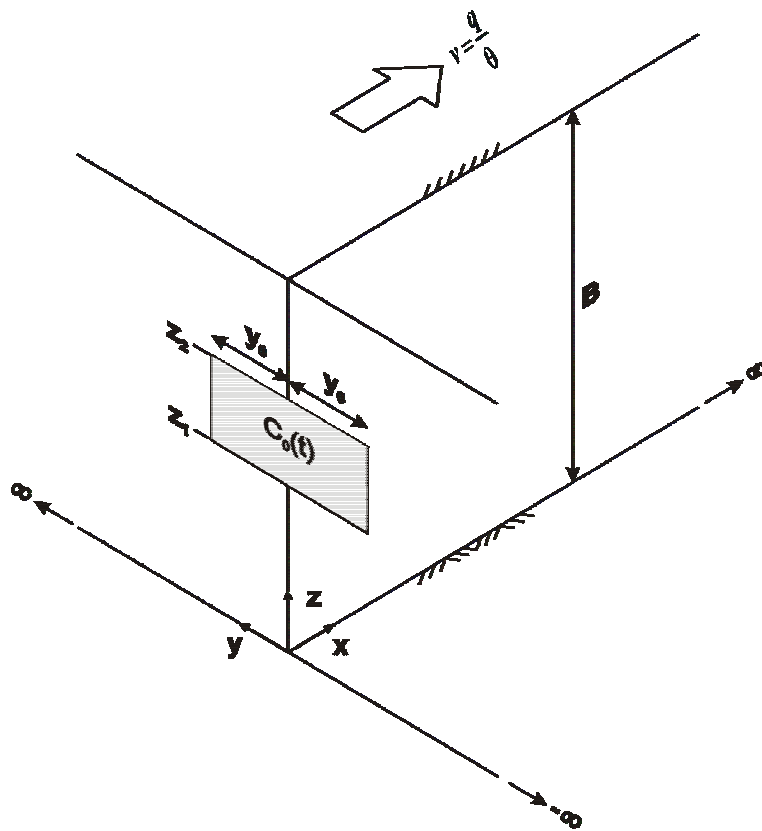


ATRANS

Analytical Solutions for Three-Dimensional Solute Transport from a Patch Source

Version 2



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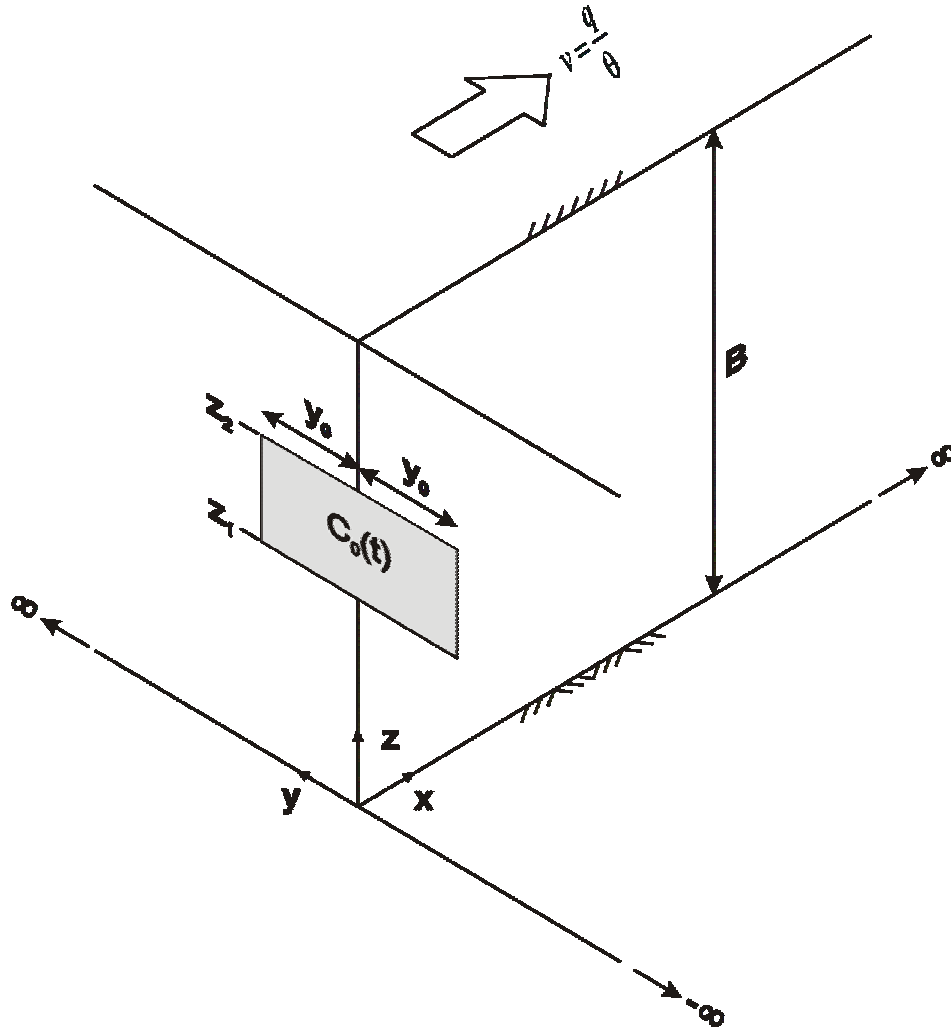
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Appendix A: Analytical Solutions for 3^D Patch Source Problem

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1. Conceptual Model

ATRANS simulates transient, three-dimensional advective-dispersive transport from a patch of specified concentration along the inflow boundary of an aquifer. The conceptual model is illustrated below. The assumptions that underlie the analytical solutions are summarized on the next page.



1.1. Dimensions

- The aquifer is semi-infinite in the longitudinal direction ($0 \leq x < \infty$);
- The aquifer is infinite in the horizontal transverse direction ($-\infty < y < \infty$); and
- The aquifer is finite in the vertical direction ($0 \leq z \leq B$).

1.2. Flow Field

- Ground water flow is steady; and
- Flow is uniform and one-dimensional along the x-axis.

1.3. Transport processes

- The following transport processes are considered: advection, dispersion, transformation reactions, and sorption;
- Dispersion is assumed to be a Fickian process;
- The principal axes of the dispersion tensor are assumed to coincide with the directions parallel and transverse to ground water flow;
- Transformation reactions are represented by a first-order decay/production reaction; and
- Sorption is assumed to be instantaneous and reversible, governed by a linear isotherm.

1.4. Initial and boundary conditions

- The aquifer is initially devoid of contaminants;
- Contaminants enter the aquifer through a rectangular patch source of specified concentration located on the upstream boundary. The concentration on the remaining portion of the upstream boundary is zero; and
- The top and bottom boundaries ($z = 0, z = B$) are zero mass flux boundaries.

2. Mathematical Model

2.1. Governing equation

Statement of mass conservation

$$\theta \frac{\partial c}{\partial t} + \rho_b \frac{\partial s}{\partial t} = -q \frac{\partial c}{\partial x} + \theta D_x \frac{\partial^2 c}{\partial x^2} + \theta D_y \frac{\partial^2 c}{\partial y^2} + \theta D_z \frac{\partial^2 c}{\partial z^2} - \theta \lambda c - \rho_b \lambda s$$

; over: $0 \leq x < \infty, -\infty < y < \infty, 0 \leq z \leq B$

where:

- c = dissolved concentration [M solute/ L³ water];
- s = sorbed concentration [M solute/ M solids];
- x, y, z = spatial coordinates [L]; and
- t = time [T].
- θ = saturated water content [L³ water/ L³ porous medium];
- ρ_b = bulk density [M solids/ L³ porous medium];
- q = Darcy flux [L/ T];
- D_x, D_y, D_z = dispersion coefficients [L²/ T]; and
- λ = first-order decay coefficients [T⁻¹].

Dispersion coefficients

The dispersion coefficients are defined as the sum of mechanical dispersion and diffusion coefficients:

$$D_x = \alpha_L \frac{|q|}{\theta} + D^* = \alpha_L v + D^*$$
$$D_y = \alpha_{TH} \frac{|q|}{\theta} + D^* = \alpha_{TH} v + D^*$$
$$D_z = \alpha_{TV} \frac{|q|}{\theta} + D^* = \alpha_{TV} v + D^*$$

where:

- α_L = longitudinal dispersivity [L];
- α_{TH} = horizontal transverse dispersivity [L];
- α_{TV} = vertical transverse dispersivity [L]; and
- D^* = effective diffusion coefficient [L²/T].

Constitutive relation for sorption

For equilibrium (instantaneous, reversible) sorption governed by a linear sorption isotherm, the relation between the concentration in solution and the concentration sorbed onto the aquifer solids is written as:

$$s = K_d c$$

where K_d is the linear sorption partitioning coefficient [L^3/M].

Defining the retardation factor, R , as:

$$R = 1 + \frac{\rho_b}{\theta} K_d$$

the governing equation can be written as:

$$\theta R \frac{\partial c}{\partial t} = -q \frac{\partial c}{\partial x} + \theta D_x \frac{\partial^2 c}{\partial x^2} + \theta D_y \frac{\partial^2 c}{\partial y^2} + \theta D_z \frac{\partial^2 c}{\partial z^2} - \theta R \lambda c$$

Here it is assumed that the contaminants in the dissolved and sorbed phases decay at the same rate.

Dividing the statement of mass conservation through by θR yields:

$$\frac{\partial c}{\partial t} = -\frac{v}{R} \frac{\partial c}{\partial x} + \frac{D_x}{R} \frac{\partial^2 c}{\partial x^2} + \frac{D_y}{R} \frac{\partial^2 c}{\partial y^2} + \frac{D_z}{R} \frac{\partial^2 c}{\partial z^2} - \lambda c$$

where $v = \frac{q}{\theta}$.

Defining: $v' = \frac{v}{R}$; $D'_x = \frac{D_x}{R}$; $D'_y = \frac{D_y}{R}$; $D'_z = \frac{D_z}{R}$

The governing equation reduces to:

$$\boxed{\frac{\partial c}{\partial t} = -v' \frac{\partial c}{\partial x} + D'_x \frac{\partial^2 c}{\partial x^2} + D'_y \frac{\partial^2 c}{\partial y^2} + D'_z \frac{\partial^2 c}{\partial z^2} - \lambda c}$$

2.2. Initial and boundary conditions

Initial Conditions

Aquifer is initial devoid of contaminant

$$c(x, y, z, 0) = 0$$

Boundary conditions

x-direction: Aquifer is semi-infinite in extent in the x -direction

- $x = 0$

$$c(0, y, z, t) = c_0(t) [H(y + y_0) - H(y - y_0)] [H(z - z_1) - H(z - z_2)]$$

where:

$c_0(t)$ = arbitrary time-varying function

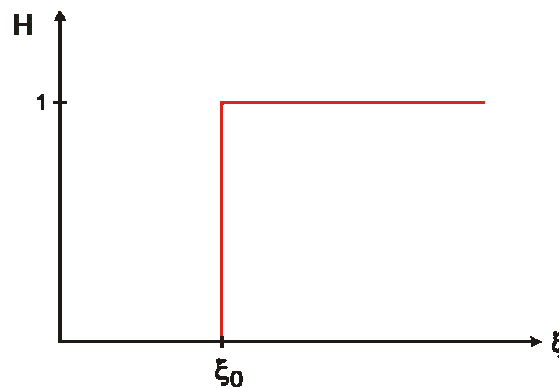
y_0 = half-width of source

z_1 = bottom of source

z_2 = top of source

$H(\cdot)$ denotes the Heaviside step function, defined as:

$$H(\xi - \xi_0) = 0 \text{ if } \xi < \xi_0 \\ = 1 \text{ if } \xi > \xi_0$$



- $x \rightarrow \infty$

$$c(\infty, y, z, t) = 0$$

y-Direction: Aquifer is infinite in extent in the y-direction

- $y \rightarrow -\infty$:

$$c(x, -\infty, z, t) = 0$$

- $y \rightarrow +\infty$:

$$c(x, \infty, z, t) = 0$$

z-Direction: Aquifer is finite in extent in the z-direction

- $z = 0$:

$$\frac{\partial c}{\partial z}(x, y, 0, t) = 0$$

- $z = B$:

$$\frac{\partial c}{\partial z}(x, y, B, t) = 0$$

where B is the thickness of the aquifer.

2.3. General solution

The general solution is derived using integral transform techniques. Complete details of the derivation are included in Appendix A. The solution is:

$$\begin{aligned}
 c = & \frac{x}{4B\sqrt{\pi D_x'}} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)} \right\} \\
 & \cdot \left[\left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D_y'(t-\tau)}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D_y'(t-\tau)}} \right\} \right] \right. \\
 & \cdot \left. \left[(z_2 - z_1) + \frac{2B}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D_z' \frac{n^2 \pi^2}{B^2} (t-\tau) \right\} \right] \right] d\tau
 \end{aligned}$$

2.4 Particular solutions for specific source concentration histories

The ATRANS package of solutions can represent four inflow concentration histories:

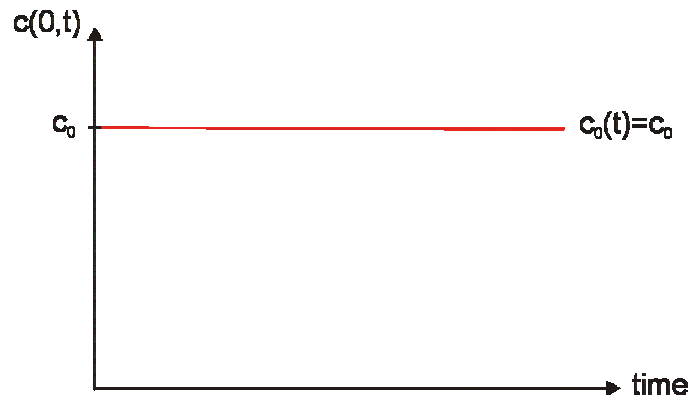
- Constant concentration;
- Exponentially-decaying concentration;
- Arbitrary inflow concentration histories represented as a set of points; and
- Arbitrary inflow concentration histories represented as a set of steps.

2.4.1 Constant concentration: ATRANS1

For a constant concentration, the boundary condition along $x = 0$ is written as:

$$c(0, y, z, t) = c_0 [H(y + y_0) - H(y - y_0)] [H(z - z_1) - H(z - z_2)]$$

which is shown as:



The solution is:

$$c = c_0 \frac{x}{4\sqrt{\pi D_x'}} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D_x' \xi} \right\} \cdot \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D_y' \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D_y' \xi}} \right\} \right] \cdot \left[\frac{(z_2 - z_1)}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D_z' \frac{n^2 \pi^2}{B^2} t \right\} \right] d\xi$$

2.4.2 Exponentially-decaying concentration: ATRANS2

For a constant concentration, the boundary condition along $x = 0$ is written as:

$$c(0, y, z, t) = c_0 \text{EXP}\{-\gamma t\} [H(y + y_0) - H(y - y_0)] [H(z - z_1) - H(z - z_2)]$$

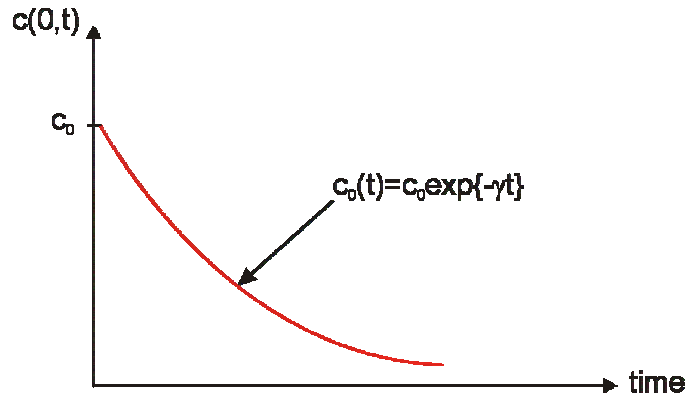
where:

γ = source decay constant [T^{-1}]

$$c_0(t) = \frac{c_0}{2} \text{ at } t = \frac{\ln 2}{\gamma}$$

The source decay constant should not be confused with the solute decay constant λ .

The inflow concentration history is illustrated below:



The solution is written as:

$$c = c_0 \frac{x}{4\sqrt{\pi D_x}} \exp\{-\gamma t\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{(\gamma - \lambda)\xi - \frac{(x - v'\xi)^2}{4D_x\xi}\right\} \cdot \left[\operatorname{erfc}\left\{\frac{y - y_0}{2\sqrt{D_y\xi}}\right\} - \operatorname{erfc}\left\{\frac{y + y_0}{2\sqrt{D_y\xi}}\right\} \right] \cdot \left[\frac{(z_2 - z_1)}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z \frac{n^2 \pi^2}{B^2} t\right\} \right] d\xi$$

2.4.3 Arbitrary time-varying concentration: ATRANS3, ATRANS4

When the inflow concentration varies arbitrarily through time, the concentration history is represented by a set of discrete steps. The inflow concentration history is written using the notation of the Heaviside step function:

$$c_0(t) = \sum_{i=1}^{NP} \Delta c_i H(t - t_i)$$

where: ΔC_i = concentration change at start of the i^{th} step

t_i = starting time of the i^{th} step

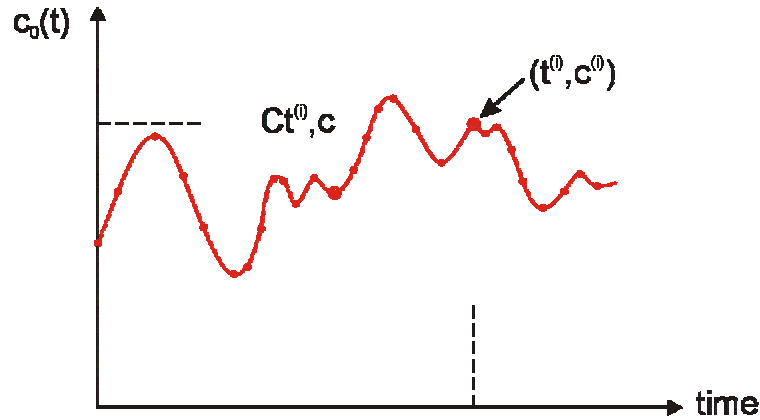
The solution for an arbitrary set of steps is given by:

$$c = \frac{x}{4\sqrt{\pi D'_x}} \sum_{i=1}^{NP} \Delta C_i \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D'_x \xi} \right\} \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D'_y \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D'_y \xi}} \right\} \right] \cdot \left[\frac{(z_2 - z_1)}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \xi \right\} \right] d\xi$$

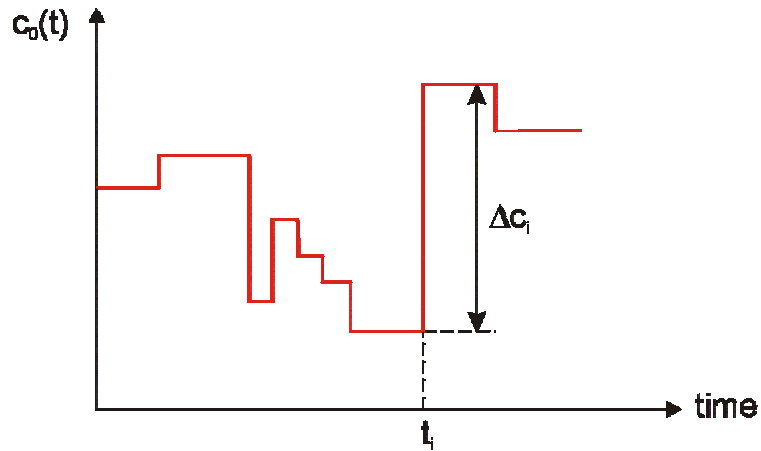
ATRANS supports two alternative approaches for representing these steps:

- Specification of a set of points, with automatic generation of the steps; or
- Direct specification of the steps.

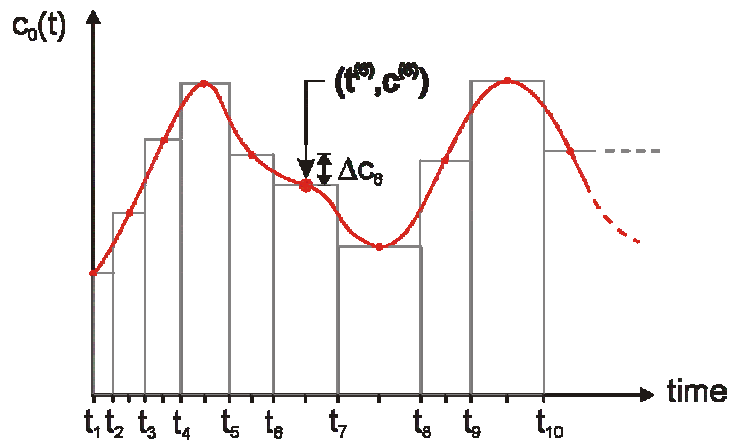
a. History specified by a set of points: **ATRANS3**



b. History specified by a set of steps: **ATRANS4**



When the inflow concentration history is specified by a set of points, ATRANS derives internally the discrete set of steps that mimics the continuous history.



The histogram is calculated according to the following rules:

$$t_n = \frac{t^{(n)} + t^{(n-1)}}{2}$$

with: $t_1 = t^{(1)} = 0$, and $\Delta C_n = c^{(n)} - c^{(n-1)}$; with $\Delta C_1 = c^{(1)}$

When the inflow concentration history is specified by a set of steps, ATRANS reads the starting times of each new concentration and calculates the concentration increment automatically.

3. ATRANS User's Guide

3.1. Installing the ATRANS codes

The ATRANS software is distributed in zipped formats (WinZip files).

We recommend that you copy the ATRANS codes and examples to a separate directory on one of your hard drives. To do this, create a new directory, for example, **C:\ATRANS**.

Extract the files using WinZip. The model subdirectories will be created automatically when the files are expanded.

If you have copied the ATRANS codes to **C:\ATRANS**, you can set the path to the ATRANS codes temporarily by typing the following from the DOS prompt (i.e., the command line):

```
C:\>set path=c:\atrans
```

You can set the path to the ATRANS codes permanently with the following steps from the Windows Start menu:

- Settings
- Control panel
- System
- Advanced
- Environment variables
- Select PATH from the environment variables
- Click edit
- Add: ;c:\ATRANS

In order for ATRANS to function properly, QuickEdit mode must be turned off.

- Activate a DOS box (Command Prompt)
- Right click anywhere along the top of the DOX box
- Properties → Options
- Uncheck the box marked “QuickEdit Mode”

If you do not want to do this every time you open a DOS-box, click on the radio button marked “Modify shortcut that started this window” when prompted to do so.

3.2. ATRANS files

ATRANS is a DOS-based program; that is, the program runs the Command Prompt.

The executable program of ATRANS was compiled using the Lahey FORTRAN 90. The program should execute without modification on IBM-compatible PCs with a 80386 CPU or higher and a math coprocessor under the DOS operating system or in the DOS compatibility mode under Microsoft *Windows*. The compiled version requires approximately 2MB extended memory to run. All of the files for ATRANS are listed below:

ATRANS1 . EXE :	executable file;
ATRANS1 . FOR :	FORTTRAN source file;
ATRANS2 . EXE :	executable file;
ATRANS2 . FOR :	FORTTRAN source file;
ATRANS3 . EXE :	executable file;
ATRANS3 . FOR :	FORTTRAN source file;
ATRANS4 . EXE :	executable file;
ATRANS4 . FOR :	FORTTRAN source file;
ATRANS . INC :	an include file for ATRANS . FOR with maximum array dimensions; and

Examples:

Example input files, located in the \EXAMPLES subdirectory.

3.3 Instructions for running the ATRANS codes

To start ATRANS, enter of the name of the program at the DOS prompt,

ATRANS1 (Constant inflow concentration)

ATRANS2 (Exponentially-decaying inflow concentration)

ATRANS3 (Inflow concentration defined by points)

ATRANS4 (Inflow concentration defined by points)

The program requires an input file to run. The input file name must have the form of *jobid*.INP where *jobid* is the base file name given by the user and .INP is the default file extension. When prompted for “a Job ID for File Specification”, enter the base name of the input file.

After the program is executed, it creates several output files with the following names where *jobid* is the same as in the input file name *jobid*.INP:

<i>jobid</i> .LST:	the echo of input parameters
<i>jobid</i> .OBS:	the listing of concentration vs. time at specified observation points
<i>jobid</i> .ASC:	an ASCII file of concentration distribution (x, y, z, c) at specified times
<i>jobid</i> .UCN:	an unformatted file of concentration distribution at specified times
<i>jobid</i> .CNF:	the model configuration file defining the computational grid for creating contour plots

3.4 ATRANS input file [*.INP file*]

The input file consists of the following records all in free format (the symbols correspond to those used in the text):

1. TITLE
2. V
3. ALX
4. ALY
5. ALZ
6. DSTAR
7. THICK
8. CLAMDA
9. R
10. NGAUS
11. NFOUR
12. SWIDTH
13. Z1
14. Z2
15. **Source history (depends on the approach adopted to represent the source history)**
16. NOBS
17. XI(1), YI(1), ZI(1) [SKIP RECORD #18 IF NOBS=0]
...
XI(NOBS), YI(NOBS), ZI(NOBS)
18. TMIN, TMAX, DELT [SKIP RECORD #19 IF NOBS=0]
19. NTIMES
20. TIME(1), ..., TIME(NTIMES) [SKIP RECORD #21 IF NTIMES=0]
22. XMIN, XMAX, DELX [SKIP RECORD #22 IF NTIMES=0]
23. YMIN, YMAX, DELY [SKIP RECORD #23 IF NTIMES=0]
24. ZMIN, ZMAX, DELZ [SKIP RECORD #24 IF NTIMES=0]

3.5 Specifying the inflow concentration history

1. ATRANS1 (Constant)

CO

2. ATRANS2 (Exponentially-decaying)

CO

SLAMDA

3. ATRANS3 (Set of points)

NP (NP must be ≥ 1)

TSI(1), CSI(1)

TSI(2), CSI(2)

...

TSI(NP), CSI(NP)

4. ATRANS4 (Set of steps)

NP (NP must be ≥ 1)

TSI(1), CSI(1)

TSI(2), CSI(2)

...

TSI(NP), CSI(NP)

Explanation of the input parameters

TITLE

A character string not to exceed 80 characters long for identification purposes.

V

The average linear groundwater velocity, v , dimension $[LT^{-1}]$.

ALX

The longitudinal dispersivity, α_L , [L].

ALY

The horizontal transverse dispersivity, α_{TH} , [L].

ALZ

The vertical transverse dispersivity, α_{TV} , [L].

DSTAR

The effective diffusion coefficient, D^* , $[L^2T^{-1}]$.

THICK

The aquifer thickness, B , [L].

CLAMDA

The first-order decay rate, λ , $[T^{-1}]$. Enter zero for a non-reactive chemical.

R

The retardation factor, R , dimensionless. Enter one for a non-reactive chemical.

NGAUS

An integer specifying the number of Gauss points used in integration (maximum 256).

NFOUR

An integer specifying the number of terms in Fourier series evaluation for partially penetrating sources. A value of 20 is normally sufficient.

SWIDTH

The total source width along the y-axis, $2y_o$, [L].

Z1

Elevation at the bottom of the source, z_1 , [L].

Z2

Elevation at the top of the source, z_2 , [L].

CO

Source concentration [ML⁻³]

SLAMDA

Source decay coefficient [T⁻¹]

NP

Number of points defining the inflow

TSI(NP) , CSI(NP)

The time and concentration at points along the source loading history profile, [T], [ML⁻³]

NOBS

The number of observation points for plotting the concentration breakthrough curves.

XI(I) , YI(I) , ZI(I)

The x, y and z coordinates of the observation points, [L], [L], [L]. The origin of the coordinate system is at the center of the patch source (see Figure 4.7 of the text).

TMIN, TMAX, DELT

The starting time, ending time, and time increment for computing concentrations at the specified observation points, [T], [T], [T].

NTIMES

The number of times at which concentration distributions are generated for the purpose of plotting contour maps.

TIME(i)

An array specifying the total elapsed times at which concentration distributions are generated. The number of values in the array TIME must be equal to NTIMES.

XMIN, XMAX, DELX

The starting coordinate, ending coordinate, and distance increment along the x axis of the computational grid used for computing the concentration distribution, [L], [L], [L],

YMIN, YMAX, DELY

The starting coordinate, ending coordinate, and distance increment along the y axis of the computational grid used for computing the concentration distribution, [L], [L], [L],

ZMIN, ZMAX, DELZ

The starting coordinate, ending coordinate, and distance increment along the z axis of the computational grid used for computing the concentration distribution, [L], [L], [L].

3.6 Postprocessing Results

3.6.1 Plotting Breakthrough Curves

Any commercial graphical package can be used to create x-y plots of concentration vs. time using the data in the *jobid*.OBS file. In this file, the first column is time, and the rest of the columns are concentrations in different observation wells arranged in order as entered in the input file.

Excerpt from an .OBS file:

0.000E+00	0.000E+00
2.500E-01	0.000E+00
5.000E-01	0.000E+00
7.500E-01	0.000E+00
1.000E+00	3.089E-16
1.250E+00	4.993E-11
1.500E+00	1.227E-07
1.750E+00	2.758E-05
2.000E+00	1.390E-03
2.250E+00	2.593E-02
2.500E+00	2.414E-01
2.750E+00	1.359E+00
3.000E+00	5.256E+00
1.450E+01	6.839E+02
1.475E+01	6.839E+02
1.500E+01	6.839E+02

3.6.2 Plotting Contour Maps

Complete concentration distributions at specified times are saved in two formats: large ASCII files listing coordinate-by-coordinate results; and compact binary files (FORTRAN-unformatted) of the same format as MODFLOW and MT3D.

ASCII Output File

Complete concentration distributions are saved in the ASCII file *jobid*.ASC, including those in different layers for a three-dimensional problem and at different times if multiple output times are specified in the input. Concentration records for different times are separated by a line specifying the time for which the following concentrations are computed. A text editor can be used to select a portion of the *jobid*.ASC file for input to a commercial contouring package such as Golden Software's *SURFER* or Spyglass' *Slicer* or *Transform*.

Excerpt from an .ASC file:

```
5.000E+00 ← time
0.000E+00      -2.000E+01      0.000E+00      0.000E+00 ← x,y,z,C
0.000E+00      -2.000E+01      2.500E-01      0.000E+00
0.000E+00      -2.000E+01      5.000E-01      0.000E+00
0.000E+00      -2.000E+01      7.500E-01      0.000E+00
0.000E+00      -2.000E+01      1.000E+00      0.000E+00
0.000E+00      -2.000E+01      1.250E+00      0.000E+00
0.000E+00      -2.000E+01      1.500E+00      0.000E+00
0.000E+00      -2.000E+01      1.750E+00      0.000E+00
```

Binary Output File

The binary output file, .UNC, is written in the following way:

```
C      write out concentration distribution to unformatted file
C      =====
      T2 = REAL(TIME(I))
      Do ilay=nz,1,-1
          LayRev=nz-ilay+1
          WRITE(65) ntrans,kstp,kper,t2,text,nx,ny,LayRev
          Write(65) (( RCONC( jj+(ii-1)*nx+(ilay-1)*nx*ny ),
&                jj=1,nx),ii=ny,1,-1)
      end do
```

This method of saving the results is consistent with the layer/row/column ordering of MODFLOW and MT3D output.

The output file is compact, but requires some postprocessing before it can be viewed with typical visualization software. Here, the PM postprocessing program is used to select results from any layer or cross section at any particular time.

PM reads the *jobid*.UCN and *jobid*.CNF files and saves data files suitable for use as input to contouring packages.

Instructions for using PM are presented in the next section.

4. PM User's Guide

4.1 Introduction

PM is used to extract the calculated concentrations within a user-specified window along a model layer or cross section at any desired time period from the unformatted concentration file saved after running *ATRANS*. The concentrations within the specified window are saved in such a form that they can be used by any commercially available graphical package to generate contour maps or other types of plots.

To use *PM*, two input files are required. The first is the unformatted file saved by *ATRANS*. The second is a text file that contains information on the spatial configuration of the model grid, referred to as the model configuration file. For output, *PM* generates data files either in the XYZ form where X and Y are the spatial coordinates of a data point and Z is the data value at (X,Y), or in the form that is directly readable by Golden Software's contouring programs *TOPO* and *SURF*.

The executable program of *PM* was compiled using the Lahey FORTRAN 77 compiler to run on IBM-compatible PCs with a 80386 CPU or higher and a math coprocessor under the DOS operating system or in the DOS compatibility mode under Microsoft *Windows*. The compiled version is based on dynamic memory allocation and will use all extended memory that is available. The executable file, *PM.EXE*, and source code of the program, *PM.FOR*, are included with the *ATRANS* software.

4.2 PM input

PM requires the existence of two files:

- Fortran unformatted concentration file; and
- Model configuration file.

Fortran unformatted file

An unformatted concentration file saved by *ATRANS* (note that the unformatted concentration file has the extensions of “.UCN”). Thus, before using *PM*, a transport simulation must have been carried out and an unformatted file saved in hard drive. The unformatted file may contain records for multiple time periods.

Model Configuration File

An input file is needed to provide *PM* with information on the spatial configuration of the model grid. This input file, referred to as **the model configuration file**, is generated automatically if *ATRANS2* has been run. A model configuration file named `jobid.CNF`, where `jobid` is the project name assigned to the simulation, is generated every time *ATRANS2* is executed. For the same project, the model configuration files created by the different programs are identical.

In the event that a model configuration file is not available, the user needs to create one manually using a text editor. The content and structure of the model configuration file is shown below:

- Record 1: NLAY, NROW, NCOL
- Record 2: (DELR(J), J=1, NCOL)
- Record 3: (DELC(I), I=1, NROW)
- Record 4: ((HTOP(J, I), J=1, NCOL), I=1, NROW)
- Record 5: (((DZ(J, I, K), J=1, NCOL), I=1, NROW), K=1, NLAY)
- Record 6: HNOFLO, [HDRV]

where

NLAY	is the total number of layers;
DELR	is the width of columns (along the row direction);
DELC	is the width of rows (along the column direction);
HTOP	is a 2D array defining the top elevation of the first model layer;
DZ	is a 3D array defining the thickness of each model cell;
HNOFLO	is the value used in the model for indicating inactive cells; and
HDRV	is the value used in the model for indicating dry cells (1.E30 by default).

Input data for the model configuration file are read using list-directed (or free) format. Therefore, each record should begin at a new line and a record can occupy as many lines as needed. Either blank spaces or commas can be used to separate values within a record. In addition, input by free format permits the use of a repeat count in the form, $n*d$, where n is an unsigned-non-zero integer constant, and the input $n*d$ causes n consecutive values of d to be entered. HTOP is a 2D array and its input should be arranged in the order of column first, sweeping from column 1 to column NCOL along the first row; then continuing onto row 2, row 3, ..., until row NROW. DZ is a 3D array and its input for each layer should be arranged similarly to that for HTOP, starting from the first layer, then continuing onto layer 2, layer 3, ..., until layer NLAY. Note that HTOP and DZ are only needed to create data files along cross sections. If one is only interested in creating data files for layers in plan view, then HTOP and DZ are never used and, thus, may be entered as dummy numbers with the use of repeat counts.

4.3 Running PM

PM can be run in either interactive or batch mode. To run it interactively, simply type the name of the executable file at the DOS prompt:

```
PM
```

The program will prompt the user for the various input items and the user responds to the input requests directly from the keyboard. To run *PM* in batch mode, write all responses in the order required by *PM* to a text file and then re-direct *PM* to get responses from the response file instead of the keyboard by issuing a command as follows:

```
PM < response file
```

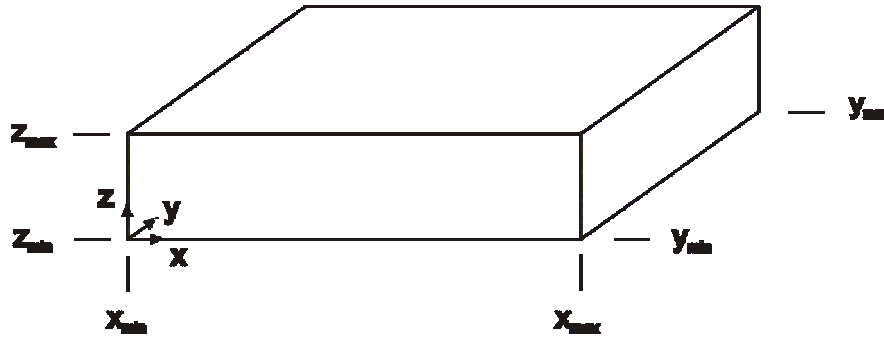
where `response file` is the name of the text file containing all responses to *PM* which the user would otherwise type in from the keyboard. Examples of the *PM* response file named `pm.ini` are included with the examples in distribution software.

The user can select the concentrations at a desired time. A value of `-1` may be entered to obtain the results at the final time period stored in the unformatted file.

4.4 Coordinate Systems for ATRANS and PM

ATRANS

ATRANS calculates the solution at specified x , y , z coordinates. The coordinates are located in a uniform Cartesian grid, defined by the limits $x_{\min} \div x_{\max}$; $y_{\min} \div y_{\max}$; and $z_{\min} \div z_{\max}$.



In addition to specifying the coordinate limits x_{\min} , x_{\max} , y_{\min} , y_{\max} , z_{\min} , z_{\max} , the user specifies the distance increments along each axis; $DELX$, $DELY$, $DELZ$.

The x , y , z coordinates of the calculation points are calculated according to:

$$\text{i) } x(j) = x_{\min} + DELX \cdot (j-1); \quad j = 1 \rightarrow NX$$

$$\text{where } NX = IDINT\left(\frac{x_{\max} - x_{\min}}{DELX} + 0.5\right) + 1$$

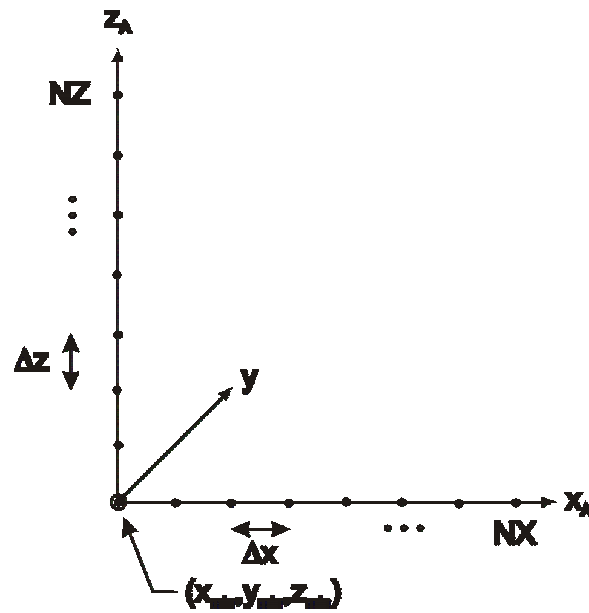
$$\text{ii) } y(i) = y_{\min} + DELY \cdot (i-1); \quad i = 1 \rightarrow NY$$

$$\text{where } NY = IDINT\left(\frac{y_{\max} - y_{\min}}{DELY} + 0.5\right) + 1$$

$$\text{iii) } z(k) = z_{\min} + DELZ \cdot (k-1); \quad k = 1 \rightarrow NZ$$

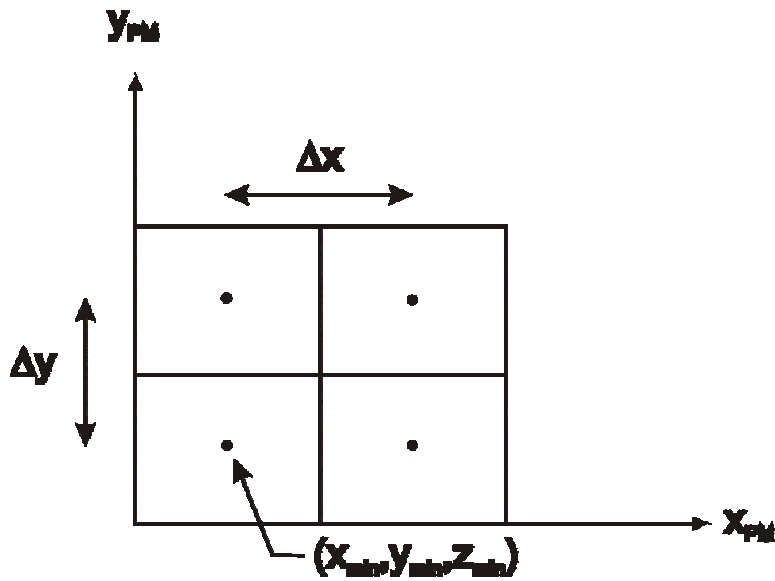
$$\text{where } NZ = IDINT\left(\frac{z_{\max} - z_{\min}}{DELZ} + 0.5\right) + 1$$

The grid points are located starting from the lower left-hand corner, as shown below:



PM

In contrast, PM assures that the coordinates are associated with a block-centered finite difference grid:

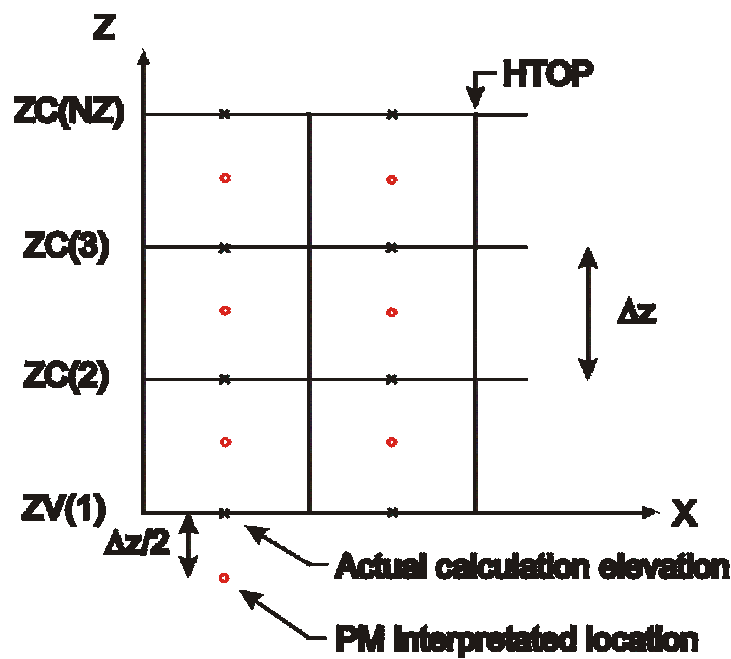


To make the ATRANS and PM coordinates coincide, it is necessary to supply PM with an offset of the coordinate origin.

Origin coordinate	x_{ATRANS}	x_{PM}	Required PM offset
x	x_{min}	$\frac{\Delta x}{2}$	$x_{\text{min}} - \frac{\Delta x}{2}$
y	y_{min}	$\frac{\Delta y}{2}$	$y_{\text{min}} - \frac{\Delta y}{2}$

A vertical offset is also required because ATRANS2 creates a model configuration file (.CNF) with the following information:

$$HTOP = ZC(NZ) \text{ and } \Delta Z$$



To match the PM interpretation to the actual calculation elevations the following vertical offset must be specified:

$$z_0 = + \frac{\Delta z}{2}$$

4.5 Output files

For output, *PM* writes data files in one of the two formats, referred to as the **.GRD** format and the **.DAT** (XYZ) format, using the conventions of Golden Software's *SURFER* graphical contouring package. The **.GRD** format as listed below writes the heads, drawdowns, or concentrations within a user-defined window of **regular** model mesh spacing to an output file, directly usable for generating contour maps by a contouring program such as the *TOPO* and *SURF* programs included in *SURFER*. Note that if heads, drawdowns or concentrations in an **irregular** portion of the model mesh are written to a **.GRD** file, no interpolation is performed and the contour map is thus deformed. The **.DAT** format as listed below writes heads, drawdowns, or concentrations at each nodal point with nodal coordinates within the user-defined window to the output file. This format is useful for generating data files of irregular model mesh spacing to be used by a gridding program such as the *GRID* program included in *SURFER* or *INTERP* included with this companion disk. It is also useful for generating plots of heads, drawdowns, or concentrations versus distances along a column, row or layer at a selected time. The **.GRD** and **.DAT** formats are listed below for reference:

(1) The “**.GRD**” file format (saved in free format):

```
DSAA
NX, NY, XMIN, XMAX, YMIN, YMAX, HMIN, HMAX
HWIN(NX, NY)
```

where:

DSAA is the character string identifying the non-binary **.GRD** format;
NX is the number of nodal points in the horizontal direction of the window;
NY is the number of nodal points in the vertical direction of the window;
XMIN is the minimum nodal coordinate in the horizontal direction of the window;
XMAX is the maximum nodal coordinate in the horizontal direction of the window;
YMIN is the minimum nodal coordinate in the vertical direction of the window;
YMAX is the maximum nodal coordinate in the vertical direction of the window;
HMIN is the minimum data value within the window;
HMAX is the maximum data value within the window; and
HWIN is a 2D array containing all data values within the window.

(2) The “.DAT” file format (saved in free format):

For each active cell inside the specified window:

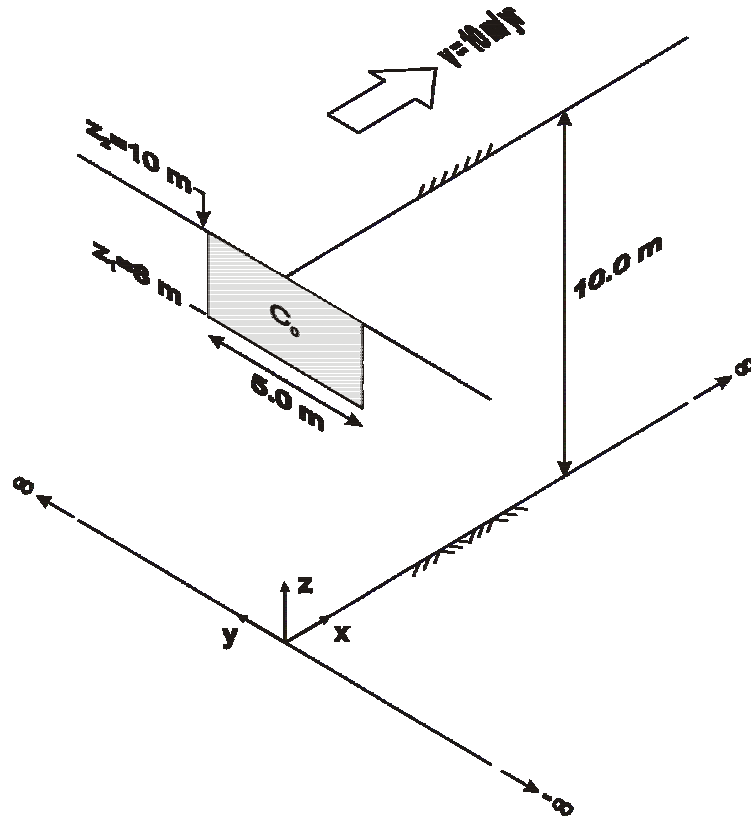
X, Y, HXY

where:

X is the nodal coordinate in the horizontal direction of the window;
Y is the nodal coordinate in the vertical direction of the window; and
HXY is the data value at the nodal point defined by (X,Y).

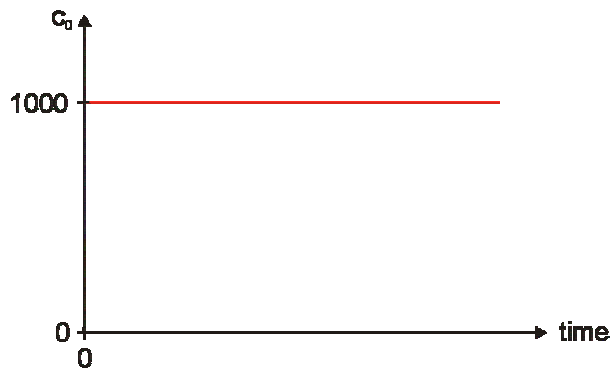
5. ATRANS Examples

5.1 Continuous Release



$$\begin{array}{ll} \alpha_L = 1.0 \text{ m} & D^* = 0 \\ \alpha_{TH} = 0.05 \text{ m} & R = 1 \\ \alpha_{TV} = 0.005 \text{ m} & \lambda = 0 \end{array}$$

Source History:



Solutions:

The solution can be calculated most simply using the code for a constant source concentration, ATRANS1. However, all four codes can be used for this problem. Example input files for the same problem for all four codes have been included to demonstrate their use.

1. ATRANS1

$$c_0 = 1000.0$$

2. ATRANS2

$$c_0 = 1000.0$$

$$\gamma = 0.0$$

3. ATRANS3, ATRANS4

$$NP = 1$$

$$t^{(1)} = 0.0; c^{(1)} = 1000.0$$

Example 1 input file: EX_1.INP

```
EXAMPLE 1
10.000
1.000
0.050
0.005
0.000
10.000
0.000
1.000
60
50
5.000
8.000
10.000
1
0.000 1000.000
1
50.000 0.000 9.000
0.000 15.000 0.500
3
5.000 10.000 15.000
0.000 250.000 10.000
-20.000 20.000 2.000
0.000 10.000 1.000
!V
!ALX
!ALY
!ALZ
!DSTAR
!THICK
!CLAMDA
!R
!NGAUS
!NFOUR
!SWIDTH (2yo)
!Z1
!Z2
!NP
!TSI(1),CSI(1)
!NOBS
!XI(1),YI(1),ZI(1)
!TMIN,TMAX,DELT
!NTIMES
!TIMES
!XMIN,XMAX,DX
!YMIN,YMAX,DY
!ZMIN,ZMAX,DZ
```

Example 1 listing file: EX_1.LST

ATrans1

ANALYTICAL SOLUTION FOR 3-D SOLUTE TRANSPORT
FROM A PATCH SOURCE WITH CONSTANT CONCENTRATION

SEMI-INFINITE IN X: $X \geq 0$
INFINITE IN Y
FINITE IN Z: $0 \leq Z \leq L$

EXAMPLE 1 (ATRANS 1)

INPUT DATA
=====

TRANSPORT PARAMETERS

AVERAGE LINEAR GROUNDWATER VELOCITY = 1.000E+01
LONGITUDINAL DISPERSIVITY = 1.000E+00
HORIZONTAL TRANSVERSE DISPERSIVITY = 5.000E-02
VERTICAL TRANSVERSE DISPERSIVITY = 5.000E-03
EFFECTIVE DIFFUSION COEFFICIENT = 0.000E+00
AQUIFER THICKNESS = 1.000E+01

SOLUTE PROPERTIES

CONTAMINANT DECAY CONSTANT = 0.000E+00
RETARDATION FACTOR = 1.000E+00

SOLUTION PARAMETERS

NUMBER OF GAUSS POINTS = 60
NUMBER OF TERMS IN SERIES = 50

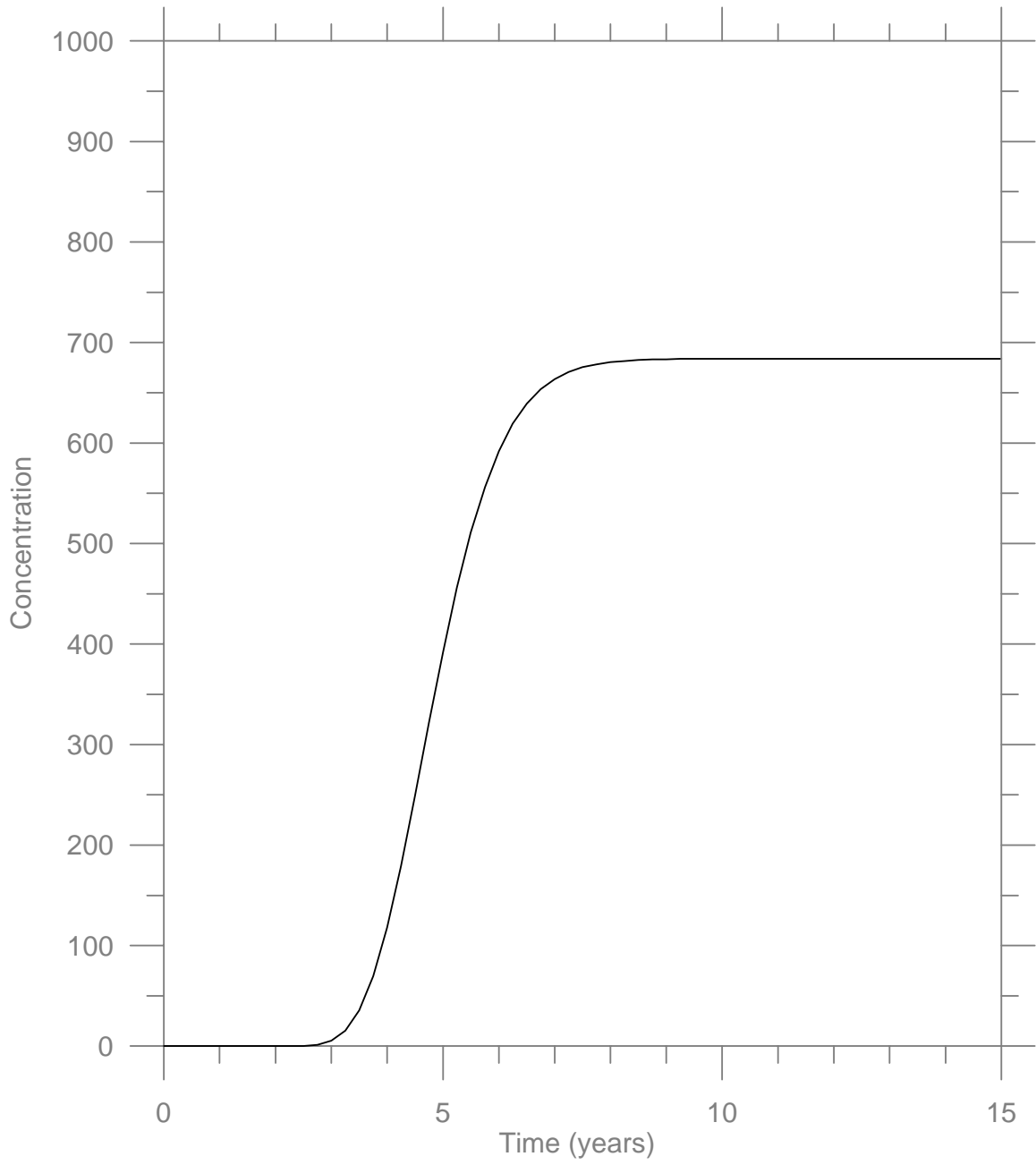
PATCH DIMENSIONS

SOURCE WIDTH = 5.000E+00
BOTTOM OF SOURCE LOCATED AT Z1 = 8.000E+00
TOP OF SOURCE LOCATED AT Z2 = 1.000E+01

INFLOW CONCENTRATION HISTORY

CONSTANT CONCENTRATION CO = 1.000E+03

Breakthrough curve at (x = 50.0 m, y= 0.0 m, z = 9.0 m)



Plan View Concentration Distribution at $z = 9.0$ m

The input file *EX_1*.INP is set up to compute complete concentration distributions at 5, 10 and 15 years. The results are extracted from the binary file of concentrations, *EX_1*.UCN, using the postprocessing program PM. Since the results are computed over a regular grid, PM can be used to generate *SURFER* GRD files directly.

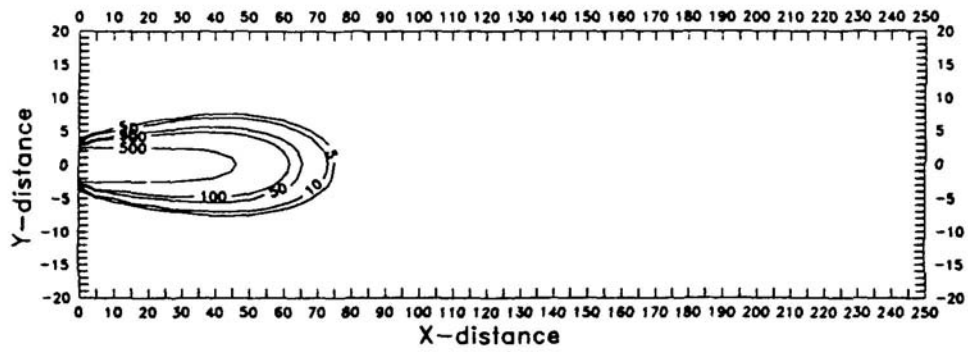
The responses to the PM prompts are given below.

PM response file: pm.fil

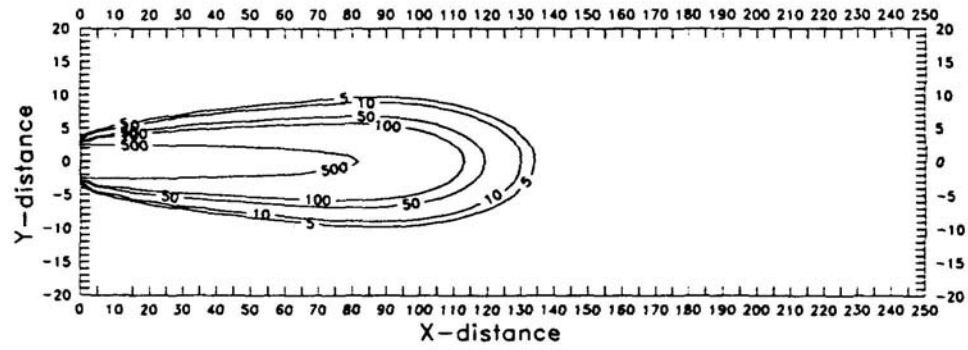
```
ex_1.ucn          ! ucn file
ex_1.cnf          ! cnf file
y                 ! offset?
-2.5,-20.5       ! xo,yo
5.                ! time
 1, 1, 5          ! j1,i1,k1
51,41, 5         ! j2,i2,k2
t5p.grd          ! output file name
1                 ! GRD format
y                 ! another plot?
y                 ! change time?
10.              ! time
n                 ! change cell indices?
t10p.grd         ! output file name
1                 ! GRD format
y                 ! another plot?
y                 ! change time?
15.              ! time
n                 ! change cell indices?
t15p.grd         ! output file name
1                 ! GRD format
n                 ! another plot?
```

Plots of the concentration distributions are shown in the next page.

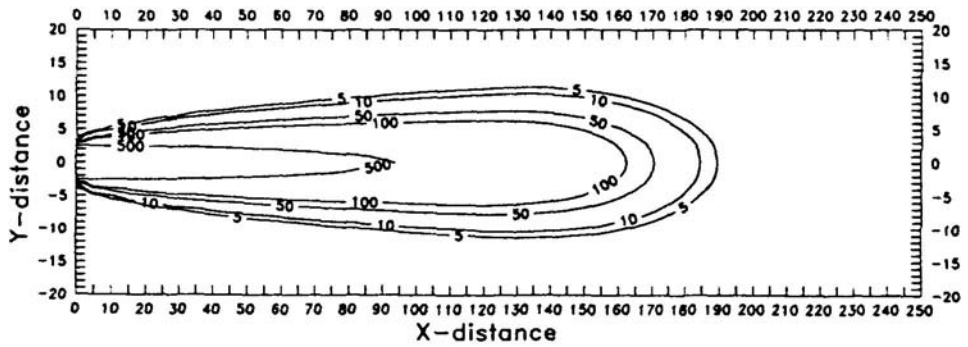
EX 1: Concentrations at $z=9.0$, $t=5$



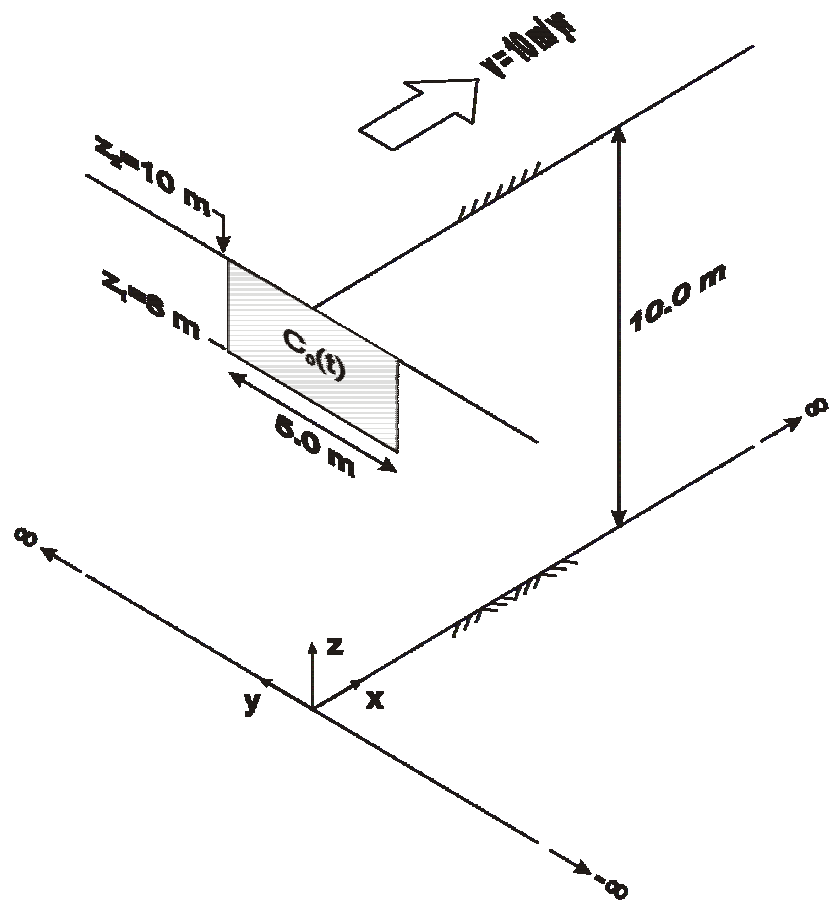
EX 1: Concentrations at $z=9.0$, $t=10$



EX 1: Concentrations at $z=9.0$, $t=15$



5.2 Finite Release



$$\begin{array}{ll} \alpha_L = 1.0\text{ m} & D^* = 0 \\ \alpha_{TH} = 0.05\text{ m} & R = 1 \\ \alpha_{TV} = 0.005\text{ m} & \lambda = 0 \end{array}$$

Source History:



Solutions: 2 Alternative approaches, ATRANS3 or ATRANS4

The solution can be calculated most simply using the code for a set of steps, ATRANS4, but it can also be obtained using the code ATRANS3. Example input files for the same problem with the two codes are included to demonstrate their use.

1. ATRANS3:

The discrete points are specified that yield the desired steps.

NP = 2:

$t^{(i)}$	$c^{(i)}$
0.0	1000.0
10.0	0.0

Note that $t^{(2)}$ is calculated from a knowledge of when the steps are to occur, and the rule for calculating the starting times of the steps.

i.e., $t^{(2)} = 2t_2 - t^{(1)}$ [from rearranging $t_2 = \frac{t^{(1)} + t^{(2)}}{2}$]

with $t^{(1)} = t_1 = 0.0$; the start of the first step and $t_2 = 5.0$; the start of the second step.

2. ATRANS4

The discrete steps in the inflow concentration are specified directly:

NP = 2:

$ts_{(i)}$	$c_{(i)}$
0.0	1000.0
x5.0	0.0

Example 2 input file: EX_2.INP

```
EXAMPLE 2
10.000
1.000
0.050
0.005
0.000
10.000
0.000
1.000
60
50
5.000
8.000
10.000
2
0.000 1000.000
10.000 0.000
1
50.000 0.000 9.000
0.000 15.000 0.250
3
5.000 10.000 15.000
0.000 250.000 5.000
-20.000 20.000 1.000
0.000 10.000 0.250

!V
!ALX
!ALY
!ALZ
!DSTAR
!THICK
!CLAMDA
!R
!NGAUS
!NFOUR
!SWIDTH (2yo)
!Z1
!Z2
!NP
!TSI(1),CSI(1)
!NOBS
!XI(1),YI(1),ZI(1)
!TMIN,TMAX,DELT
!NTIMES
!TIMES
!XMIN,XMAX,DX
!YMIN,YMAX,DY
!ZMIN,ZMAX,DZ
```

Example 2 listing file: EX_2.LST

```
ATrans4
*****
ANALYTICAL SOLUTION FOR 3-D SOLUTE TRANSPORT
FROM A PATCH SOURCE WITH TIME-VARYING CONCENTRATION

SEMI-INFINITE IN X: X>=0
INFINITE IN Y
FINITE IN Z: 0<=Z<=L

EXAMPLE 2: atrans4

INPUT DATA
=====

TRANSPORT PARAMETERS
-----
AVERAGE LINEAR GROUNDWATER VELOCITY = 1.000E+01
LONGITUDINAL DISPERSIVITY = 1.000E+00
HORIZONTAL TRANSVERSE DISPERSIVITY = 5.000E-02
VERTICAL TRANSVERSE DISPERSIVITY = 5.000E-03
EFFECTIVE DIFFUSION COEFFICIENT = 0.000E+00
AQUIFER THICKNESS = 1.000E+01

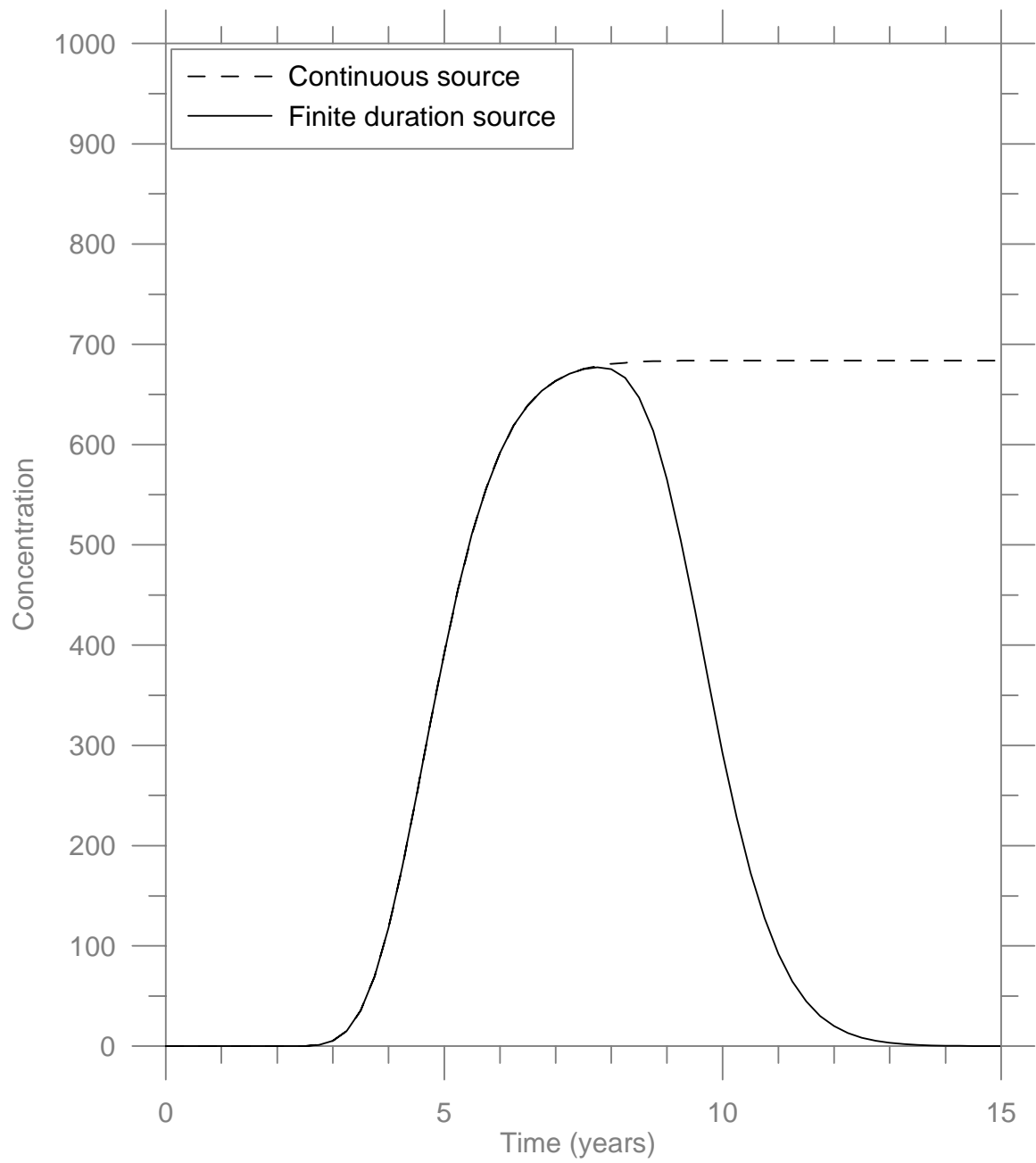
SOLUTE PROPERTIES
-----
CONTAMINANT DECAY CONSTANT = 0.000E+00
RETARDATION FACTOR = 1.000E+00

SOLUTION PARAMETERS
-----
NUMBER OF GAUSS POINTS = 60
NUMBER OF TERMS IN SERIES = 50

PATCH DIMENSIONS
-----
SOURCE WIDTH = 5.000E+00
BOTTOM OF SOURCE LOCATED AT Z1 = 8.000E+00
TOP OF SOURCE LOCATED AT Z2 = 1.000E+01

SPECIFIED INFLOW CONC. HISTOGRAM
=====
START OF INTERVAL          CONCENTRATION
0.000E+00                  1.000E+03
5.000E+00                  0.000E+00
```

Breakthrough curve at (x = 50.0 m, y= 0.0 m, z = 9.0 m)



5.3 Decaying source

Parameters:

Average linear groundwater velocity, v :	10.0 m/yr
Longitudinal dispersivity, α_L :	1.0 m
Horizontal transverse dispersivity, α_{TH} :	0.05 m
Vertical transverse dispersivity, α_{TV} :	0.005 m
Effective molecular diffusion coefficient, D^* :	0.0
First-order decay coefficient, λ :	0.0
Retardation factor, R :	1.0
Aquifer thickness, B :	10.0 m
Bottom elevation of source top, z_1 :	8.0 m
Top elevation of source top, z_2 :	10.0 m
Source width, $2y_0$:	5.0 m

Source history:

$$c(0, t) = c_0 \text{EXP}\{-\gamma t\}$$

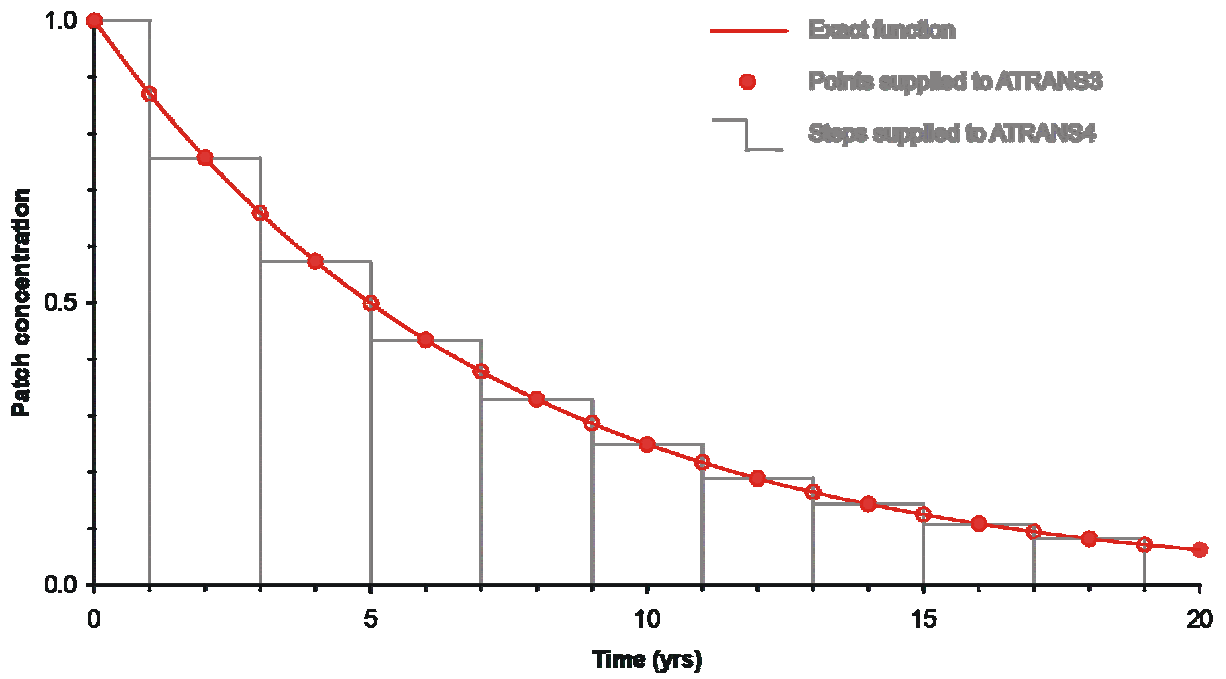
Initial concentration, c_0 :	1.0
Source decay coefficient, γ :	0.139 yr ⁻¹

Solutions:

The solution can be calculated most simply using the code for an exponentially decaying source, ATRANS2. However, the solution can also be obtained with discrete representations of the source as a set of steps, ATRANS4, or a set of points, ATRANS3. Example input files for the same problem with the two codes are included to demonstrate their use.

1. ATRANS2
 $c_0 = 1000.0$
 $\gamma = 0.139$

- 2. ATRANS3 – 11 points specified
ATTRANS4 – 11 steps specified



Example 3 input file: EX_3.INP

```

EXAMPLE 3: atrans3
10.000
 1.000
 0.050
 0.005
 0.000
10.000
 0.000
 1.000
 60
 50
 5.000
 8.000
10.000
11
 0.0 1.0000
 2.0 0.7579
 4.0 0.5744
 6.0 0.4354
 8.0 0.3300
10.0 0.2501
12.0 0.1895
14.0 0.1436
16.0 0.1089
18.0 0.0825
20.0 0.0625
 1
50.000 0.000 9.000
 0.000 15.000 0.100
 1
10.000
 0.000 150.000 5.000
 0.000 0.000 1.000
 9.000 9.000 1.000
!V
!ALX
!ALY
!ALZ
!DSTAR
!THICK
!LAMDA
!R
!NGAUS
!NFOUR
!SWIDTH (2yo)
!Z1
!Z2
!NP
!TI(1),CI(1)
!NOBS
!NTIMES
!TIMES
!XMIN,XMAX,DX
!YMIN,YMAX,DY
!ZMIN,ZMAX,DZ

```

Example 3 listing file: EX_3.LST

```
ATrans3
*****
ANALYTICAL SOLUTION FOR 3-D SOLUTE TRANSPORT
FROM A PATCH SOURCE WITH TIME-VARYING CONCENTRATION

SEMI-INFINITE IN X: X>=0
INFINITE IN Y
FINITE IN Z: 0<=Z<=L

EXAMPLE 3: atrans3

INPUT DATA
=====

TRANSPORT PARAMETERS
-----
AVERAGE LINEAR GROUNDWATER VELOCITY = 1.000E+01
LONGITUDINAL DISPERSIVITY           = 1.000E+00
HORIZONTAL TRANSVERSE DISPERSIVITY  = 5.000E-02
VERTICAL TRANSVERSE DISPERSIVITY    = 5.000E-03
EFFECTIVE DIFFUSION COEFFICIENT     = 0.000E+00
AQUIFER THICKNESS                   = 1.000E+01

SOLUTE PROPERTIES
-----
CONTAMINANT DECAY CONSTANT          = 0.000E+00
RETARDATION FACTOR                  = 1.000E+00

SOLUTION PARAMETERS
-----
NUMBER OF GAUSS POINTS              = 60
NUMBER OF TERMS IN SERIES           = 50

PATCH DIMENSIONS
-----
SOURCE WIDTH                         = 5.000E+00
BOTTOM OF SOURCE LOCATED AT Z1      = 8.000E+00
TOP OF SOURCE LOCATED AT Z2        = 1.000E+01
```

INFLOW CONCENTRATION HISTORY

```

-----
      TIME          CONCENTRATION
0.000E+00      1.000E+00
2.000E+00      7.579E-01
4.000E+00      5.744E-01
6.000E+00      4.354E-01
8.000E+00      3.300E-01
1.000E+01      2.501E-01
1.200E+01      1.895E-01
1.400E+01      1.436E-01
1.600E+01      1.089E-01
1.800E+01      8.250E-02
2.000E+01      6.250E-02
    
```

CONSTRUCTED INFLOW CONC. HISTOGRAM

```

=====
      TIME INTERVAL          CONCENTRATION
0.000E+00 - 1.000E+00      1.000E+00
1.000E+00 - 3.000E+00      7.579E-01
3.000E+00 - 5.000E+00      5.744E-01
5.000E+00 - 7.000E+00      4.354E-01
7.000E+00 - 9.000E+00      3.300E-01
9.000E+00 - 1.100E+01      2.501E-01
1.100E+01 - 1.300E+01      1.895E-01
1.300E+01 - 1.500E+01      1.436E-01
1.500E+01 - 1.700E+01      1.089E-01
1.700E+01 - 1.900E+01      8.250E-02
1.900E+01 --> INFINITY      6.250E-02
    
```


Breakthrough curve at (x = 50.0 m, y= 0.0 m, z = 9.0 m)

