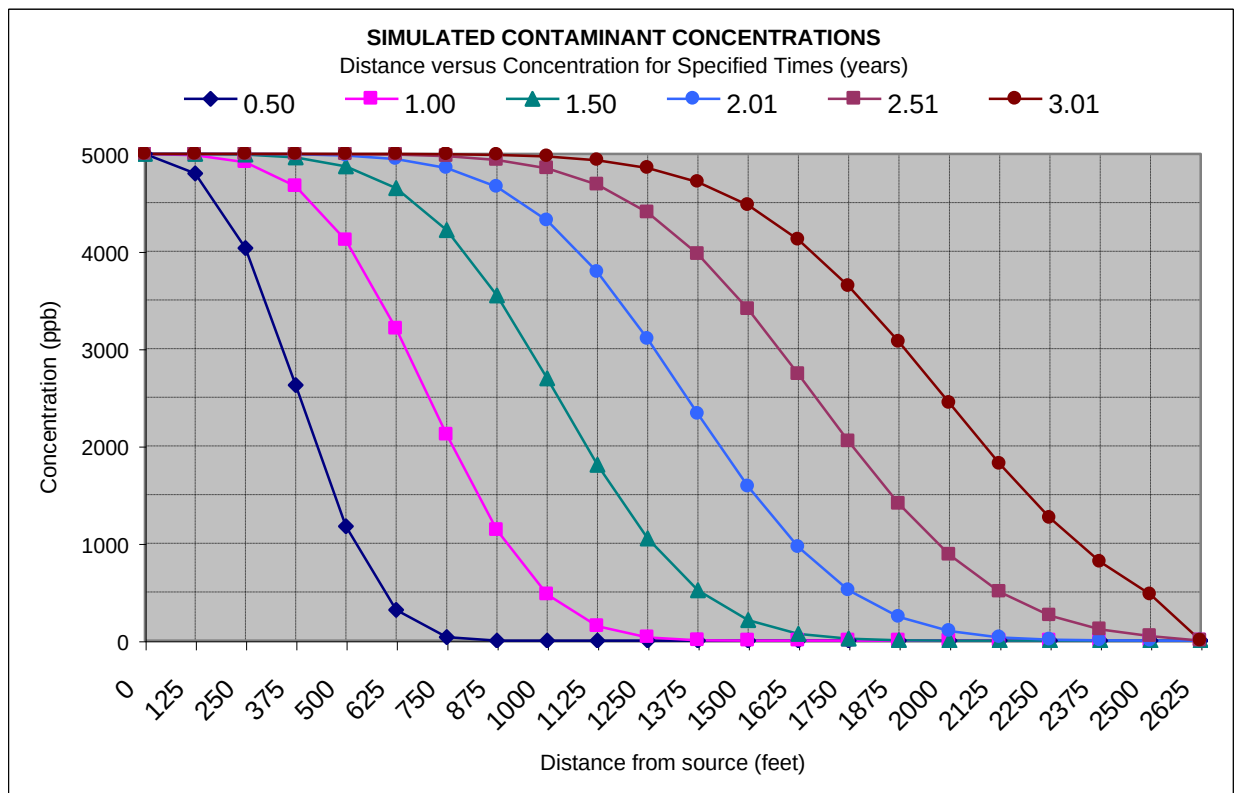


Woburn 1-D Contaminant Transport Game

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Introduction

The Woburn 1-D Contaminant Transport Game is an EXCEL spreadsheet that enables the user to compute concentrations of TCE traveling in the groundwater flow system toward well H that emanate from the W.R. Grace. The spreadsheet computes values of hydraulic head, advective flow velocities and traveltimes, contaminant velocities and traveltimes, and contaminant concentrations at 20 locations along the flowpath from W.R. Grace to the Aberjona River. Breakthrough curves showing changes in concentration versus distance and changes in concentration versus time pop-up automatically (see below). The spreadsheet also creates graphs of advective and contaminant velocities versus distance.



Hydrogeologic input parameters are porosity (n), aquifer thickness (b), hydraulic conductivity (K), and recharge rate in the 20 cells along the flowpath. Input values used in the finite-difference solution include the initial concentration of the contaminant at W.R. Grace (C_0), time step duration (Δt), longitudinal dispersivity (α), and chemical retardation (R_f). Suggested values of these parameters are given in Table 1.

The spreadsheet calculates differences between measured water levels in observation wells located along the flowpath with simulated heads at corresponding cells. It computes the mean absolute error between measured and simulated heads.

Actual water levels were measured in a network of observation by the U.S. Geological Survey (Myette and others, 1987). The spreadsheet also calculates the discharge (ft^3/day) along the flowpath (flow tube of width Δy) into the 21st cell, which represents the Aberjona River. This value is compared with an estimate of the streamflow gain along this segment of the Aberjona River (Δy) based on stream discharge measurements made by the U.S. Geological Survey (Myette and others, 1987). Therefore, the user has two sets of calibration targets (heads and fluxes) to measure the “goodness-of-fit” of the flow model against actual field data. The transport model cannot be calibrated because no TCE data were collected prior to closure of municipal wells G & H.

One object of the game is to minimize the difference between measured and simulated hydraulic heads and measured and simulated streamflow gain while using realistic values of aquifer thickness, hydraulic conductivity, and porosity. This enables the user to gain insight into the mass and concentration of TCE reaching the Aberjona River (the area near well H) during the period from November 1960, when the W.R. Grace plant began operation, to May 1979, when wells G & H were shutdown.

Limitations

The solution to the advection-dispersion equation used in this spreadsheet assumes that contaminant transport is transient through a steady-state, one-dimensional flow field. As a consequence of this assumption, no pumping stresses from wells G & H can be incorporated in the spreadsheet. Thus, the simulated velocity field is based on variations in hydraulic gradient between W.R. Grace and the Aberjona River produced by spatial variations in hydraulic conductivity, aquifer thickness, and recharge between the upland area and the wetland as would have existed prior to the construction well G in 1964. Changes to regional hydraulic gradients caused by the periodic operation of wells G and H between 1964 and 1979 create transient, three-dimensional flow effects that cannot be represented in a simple one-dimensional analysis.

The advection-dispersion equation is difficult to solve numerically. Peclet and Courant criteria are designed to prevent numerical errors in the solution (Anderson and Woessner, 1992). The Peclet criterion ($P_e = \Delta x / \alpha$) limits the size of grid cells relative to the magnitude of dispersivity used in the solution. Generally, P_e should be less than or equal to 1, although this spreadsheet commonly produces good results when P_e is less than or equal to 2. It is easiest to simply change the value of α used in the spreadsheet to adjust P_e . In the spreadsheet, Δx is fixed at 125 feet. Changes to Δx entail modifying the structure of the entire spreadsheet, which is difficult to implement.

The Courant criterion ($C = v_c \Delta t / \Delta x$) is designed to limit contaminant movement in each time step. This spreadsheet seems to work best when C is less than 0.7, which was determined solely by trial-and-error use. In the spreadsheet, C is adjusted by changing Δt , because Δx is fixed at 125 feet. The spreadsheet also works best when the ratio of C/P_e is less than 0.5. This value also was determined by experimentation. Adherence to these three criteria is documented in the top right corner of the spreadsheet.

Example Problem

An interesting assignment is to use the spreadsheet to approximately compare the differences in contaminant concentrations and traveltimes for the two divergent conceptualizations of the groundwater flow system presented by expert witnesses at the famous trial described in the award-winning book *A Civil Action* (Harr, 1995) and in the movie of the same name (Touchstone Pictures, 1998). One expert witness (Expert A) based his professional opinions, in part, on use of a one-dimensional analytical calculation that assumed the aquifer between W.R. Grace and the river had a uniform thickness, a uniform hydraulic conductivity, a uniform porosity, and no recharge. Another expert witness (Expert B) based his professional opinions, in part, on the results of a three-dimensional flow and transport numerical model that accounted for spatial variations in aquifer thickness, hydraulic conductivity, porosity, and recharge, among other parameters. The spreadsheet can be used to compare these two different conceptualizations in the one dimensional case and to draw conclusions as to whether the simulated results from which conceptualization are more realistic.

The file **2001gsa.xls** contains two versions of the spreadsheet program. At the bottom of the worksheet, one is labeled *W.R. Grace – heterogeneous* and represents the conceptualization of Expert B, whereas the other is labeled *W.R. Grace – homogeneous* and represents the conceptualization of Expert A. Listed below are values of relevant parameters used by each expert based largely on their trial depositions and courtroom testimony (Bair, 2001).

Table 1.
Parameter Values Used to Simulate Flow and Transport from W.R. Grace

<i>Parameter / Variable</i>	<i>Expert A</i>	<i>Expert B</i>
<i>Time step (days)</i>	36.5	73
<i>Porosity (decimal)</i>	0.25	0.20 – 0.35
<i>Hydraulic conductivity (ft/d)</i>	75	0.5 – 200
<i>Aquifer thickness (ft)</i>	20	10 - 50
<i>Recharge rate (ft/yr)</i>	0	0.5 – 2.0
<i>C_o (ppb)</i>	5000	5000
<i>R_f for TCE</i>	4.0	4.0
<i>Dispersivity (ft)</i>	67	67

The *W.R. Grace – homogeneous* spreadsheet for Expert A is set up using the parameters listed in Table 1. The results of this representation of the flow system and the transport of TCE are summarized in Table 2 below.

The parameter values in the *W.R. Grace – heterogeneous* spreadsheet are not completely consistent with the hydrogeologic data presented during the field trip. Based on the information presented during the trip, modify and improve the *W.R. Grace – heterogeneous* spreadsheet to incorporate more realistic spatial variations in

hydrogeologic parameters. Then, fill in Table 2 with the results from your simulation that produces the lowest errors between measured and simulated heads and between measured and simulated streamflow gain.

Table 2.
Comparison of Results from the Two Differing Conceptualizations of the Flow System

Point of Comparison	Expert A Simulation	Expert B Simulation
Computed mean absolute error in water levels (ft)	9.09	1.59
Computed error in streamflow gain (percent)	-144	14
Advective flow velocity at 500 ft from source (ft/d)	5.7	0.38
Contaminant flow velocity at 500 ft from source (ft/d)	1.4	0.10
Total advective traveltime to 2625 ft (yrs)	1.2	21.7
Simulated TCE concentration at 500 ft at 1 year (ppb)	3445	0
Simulated TCE concentration at 500 ft at 5 years (ppb)	4996	18
Simulated TCE concentration at 1000 ft at 2 years (ppb)	3279	0
Simulated TCE concentration at 1000 ft at 10 years (ppb)	5000	6
Simulated TCE concentration at 1000 ft at 15 years (ppb)		34
Simulated TCE concentration at 2500 ft at 2 years (ppb)	1	0
Simulated TCE concentration at 2500 ft at 10 years (ppb)	4990	0
Simulated TCE concentration at 2500 ft at 15 years (ppb)		0
Simulated TCE concentration at 2500 ft at 20 years (ppb)		2

As you can see from Table 2, based on the conceptualization and simulation of Expert A, TCE reaches the area near well H within 1 to 2 years. This suggests that the groundwater at the future sites of wells G and H along the Aberjona River was contaminated by TCE before the wells were drilled in 1964 and 1967, respectively, and therefore the water pumped by wells G and H into the municipal water mains was contaminated from October 1964 to the day the wells were closed in May 1979.

What does the conceptualization and simulation of the flow system by Expert B suggest?

Do you think a jury of non-scientists could understand the geology, hydrology, and aqueous chemistry in sufficient detail to appreciate the differences in the way these two experts conceptualized and simulated the flow system?

Using the Spreadsheet

The spreadsheet should open easily into all versions of EXCEL. In some cases, it may be necessary to reset the iterative equation solver in EXCEL. This is done by clicking on *Tools* on the Menu Bar. Select *Options*, then select *Calculation*. Once you are in the *Calculation* menu, click on *Manual*, click on *Iteration*, and set *Maximum Iterations* to 1000 and *Maximum Change* to 0.00001. Return to the spreadsheet. To start

the iterative equation solver simply hit the *F9* key on your keyboard. If your computer is slow, you may want to decrease *Maximum Iterations* to 500 and *Maximum Change* to 0.0001. This will speed up the convergence of the iterative equation solver, but it will yield a less accurate solution that produces larger errors in mass balance.

In some cases it also may be necessary to zoom in or out of the spreadsheet so the text shows in each cell. This prevents the dreaded ##### symbol from appearing in cells. To do this, select *View* on the Menu Bar. Then select *Zoom*. For most computer screens a zoom factor of 75% to 100% keeps the dreaded ##### symbol away.

If you receive an error message about a “circular reference” in one or more of the equations, ignore it. This, I think, is a consequence of using a numerical algorithm combined with the stochastic nature of any Bill Gates product.

The spreadsheets are set up so that only certain cells can be changed (*n*, *b*, *K*, Δt , α , *C_o*, *R_f*). All other cells are protected to preserve the finite-difference equations, other calculations, and graphs.

Solution Technique

For those who are interested, the 1-D advection-dispersion equation is solved using an explicit finite-difference solution incorporating chemical retardation (*R_f*)

$$R_f \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) - \frac{\partial}{\partial x} (v_x C)$$

The solution addresses contaminant transport in a steady-state, heterogeneous flow field with spatially variable recharge, where the velocity field is determined using a Poisson formulation. The concentration (*C*) at cell *i* at time step *t* is determined by

$$C_i^t = C_i^{t-1} + \frac{\Delta t}{R_f \Delta x} \left(\frac{\alpha_x v_{i+1/2} (C_{i+1}^{t-1} - C_i^{t-1}) - \alpha_x v_{i-1/2} (C_i^{t-1} - C_{i-1}^{t-1})}{\Delta x} \right) - \frac{\Delta t}{R_f \Delta x} (v_{i+1/2} C_i^{t-1} - v_{i-1/2} C_{i-1}^{t-1})$$

where $D_i = \alpha_x v_i$ is hydrodynamic dispersion (molecular diffusion is ignored) and the terms $v_{i-1/2}$ and $v_{i+1/2}$ are flow velocities at the interfaces between cells *i* and *i-1* and cells *i* and *i+1*, respectively (modified from Zheng and Bennett, 1995, p. 161). This introduces students to the concepts of stability and numerical dispersion as the solution is unstable if the Peclet and Courant constraints are not met.

The Woburn 1-D Contaminant Transport Game was conceived as a classroom assignment in one of my numerical modeling courses. The original EXCEL spreadsheet has been revised several times since then. A description of the use of spreadsheets in teaching groundwater flow modeling techniques to students can be found in Anderson and Bair (2001).

The spreadsheet is not foolproof by any means. Certain combinations of parameter values can produce bizarre results. For example, adding too much recharge on the upland can cause a reversal of groundwater flow directions, which creates a local groundwater divide in the flow field. This, in turn, causes the transport algorithm to produce some truly wild results. In reality, there is no local groundwater divide between W.R. Grace and the Aberjona. My guidance is that if you keep the groundwater flow components realistic, the transport algorithm should do fine. Under some combinations of parameters the downgradient boundary conditions used to remove contaminant mass in the 21st cell does not work. I have no solution for this at present and welcome any suggestions.

References

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