Using the Domenico Solution to Teach Contaminant Transport Modeling

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ABSTRACT

The Domenico solution is a heuristic simplification of a solution to the transport equation. Although there is a growing consensus that the Domenico solution is undesirable for use in professional and research applications due to departures from exact solutions under certain conditions, it behaves well under conditions suitable for instruction. Moreover, the solution is easily programmed into spreadsheets, and incorporated into classroom exercises that illustrate the basic processes of advection, dispersion, retardation, evaluation of the error and complimentary error functions, sensitivity analyses, and Monte Carlo simulations. Exercises of these kinds provide students in introductory (e.g., students with no previous exposure to the subject) or intermediate courses (e.g., students having completed previous, related course work) with bottom-up experience preparing models, without a full commitment to learning a programming language. This frees the students to spend more time learning the physical processes, the parameter relationships, and experiencing the steps of moving from the equations to a computer code. A student survey and an instructor evaluation of a class project (class of 11 students) both indicated success in student learning at the levels desired for the course. © *2012 National Association of Geoscience Teachers*. [DOI: 10.5408/11-230.1]

Key words: Domenico solution, contaminant transport, spreadsheet, error function, advection-dispersion equation, dispersion, Monte Carlo

INTRODUCTION

The goal of this paper is to show that a heuristic simplification of an analytical solution to the advection-dispersion equation with sorption and reaction terms (hereafter referred to as the transport equation) can be used to instruct students in introductory or intermediate classes in groundwater contaminant transport. To achieve this we show that the simplification comes with advantages that make it a reasonable alternative to exact solutions for simulations representative of some realistic scenarios. Finally, we present the results of a student survey and an assessment of student work to show the effectiveness of the instruction. The basis for the exercises presented here is an equation commonly known as the Domenico solution (Domenico, 1987).

According to Hepburn (2011) there are few published teaching exercises on groundwater modeling, though resources on which such exercises can be built have been available for several years (for example see Li and Liu, 2003). In our experience, there are still fewer resources available for transport modeling education, a need addressed in this article. Using the Domenico solution, we outline exercises to illustrate basic transport principles in a spreadsheet environment. Spreadsheets are widely available and therefore constitute an ideal platform for instruction in transport modeling (Bair and Lahm, 2006).

In order to teach contaminant transport to students with limited background on the subject, our approach is to demystify the equations by enabling students to code them, and to build an intuitive understanding of the processes by linking the terms in the transport equation (Eq. 1) to physical changes in plume size and shape. The transport equation can be written

$$R\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} - v\frac{\partial C}{\partial x} - \lambda C, \qquad (1)$$

where x, y, and z are distances in the three spatial directions (L), R is a dimensionless retardation factor, C is concentration (M/L^2), D is a dispersion coefficient (L^2/T) ($= \alpha_{x,y,z}v + D^*$), $\alpha_{x,y,z}$ is dispersivity in the direction indicated by the subscript x,y, or z (L), v is average linear velocity in the x direction (direction of water flow)(L/T), D^* is an effective diffusion coefficient (L^2/T), and λ is a pseudo-first-order rate constant (T^{-1}). Units are presented in generalized form with M representing mass, L length, and T time.

Analytical solutions are exact solutions to differential equations, in contrast to numerical solutions, which are approximations and involve time and space stepping. Analytical solutions offer the advantages of fast execution and straightforward parameterization compared to numerical solutions like MODFLOW and MT3D, the commonly used USGS flow and transport codes, respectively. In a spreadsheet environment, students can quickly and easily program many analytical solutions, empowering them to apply the mathematics beyond the course. They can vary the input values of analytical solutions and almost instantly see the output expressed graphically. The rapid feedback facilitates digital experimentation and the development of an intuitive sense of how parameters like dispersivity, retardation factors, and rate constants influence plume shape and size. To maximize the learning potential of this

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tool, experimentation with a three-dimensional (3D) plume model is preferred.

Since its introduction in 1987, the 3D Domenico solution has been widely used by regulators, practitioners, and researchers due its ease of use and analytical origin (Newell et al., 1996; McNab and Dooher, 1998; Khan and Husain, 2003; Atteia and Guillot, 2007). However, the lack of mathematical rigor in its derivation has raised questions about its accuracy with differing conclusions about its suitability for continued use (Guyonnet and Neville 2004, West et al., 2007, Srinivasan et al., 2007). Therefore, before continuing with a series of exercises that use the Domenico solution, it is best to re-evaluate it for the purposes of instruction. First, it is worth noting that the strongest argument against use of the Domenico solution is that modern computers and readily available software can provide users with exact solutions or well established numerical models so, the argument goes, there is no justification for using anything less. This position has particular merit where decisions of weight with financial or environmental consequences depend on the modeling result. However, when used appropriately in preliminary calculations or for the purposes of instruction, the Domenico solution offers advantages, discussed below, that establish it as a useful tool.

Usefulness of the Domenico Solution

The statistician George E. P. Box wrote, "For . . . a model there is no need to ask the question 'is the model true?' If 'truth' is to be the 'whole truth' the answer must be 'No.' The only question of interest is 'Is the model illuminating and useful?' " (Box, 1979, p. 3). There can be little doubt that the highest standards for groundwater models require the constituent equations to be rigorously derived and correct, for example see Sagar (1982) or Wexler (1992) (hereafter referred to as the Sagar/Wexler solution). Nevertheless, it must be remembered that even these models incorporate simplifying assumptions that limit their ability to accurately represent transport in aquifers. If the approximate Domenico solution returns concentration output within the uncertainty range of the exact solution, it might be regarded as a useful screening level tool. This argument is the basis of the third teaching exercise described in this article.

ASSESSMENT OF THE DOMENICO SOLUTION

Before moving on to the teaching exercises, it is desirable to see the Domenico solution, and how it differs from the exact Sagar/Wexler solution. Although not developed here as an exercise, this information could be adapted by readers for teaching purposes.

The Solutions

The Domenico and Sagar/Wexler solutions solve the equation subject to the following boundary conditions. A rectangular source located at $x = 0$ is assumed with a constant concentration of C_o (M/L^3). The source is centered at $y = 0$ with a total width of Y. The top of the source is assumed to coincide with the top of the domain and extends downward to a depth of Z. The concentration of the solute everywhere downstream of the source at time = 0 is assumed 0, and the concentration at $x = y = z = \infty$ is assumed 0 at all time.

The Domenico solution may be written (Domenico, 1987; Wang and Wu, 2009),

$$
\begin{aligned}
\frac{C}{C_o} = \frac{1}{8}\exp\left[\frac{vx}{2D_x}\left[1-\left(1+\frac{4\lambda D_x}{v^2}\right)^{0.5}\right]\right] \\
\times erfc\left[\frac{x - vt\sqrt{1+4\lambda D_x/v^2}}{2\sqrt{\alpha_x vt}}\right] \\
\times\left\{erf\left[\frac{y+\frac{Y}{2}}{2\sqrt{\frac{D_y x}{v}}}\right] - erf\left[\frac{y-\frac{Y}{2}}{2\sqrt{\frac{D_y x}{v}}}\right]\right\} \\
\times\left\{erf\left[\frac{z+Z}{2\sqrt{\frac{D_z x}{v}}}\right] - erf\left[\frac{z-Z}{2\sqrt{\frac{D_z x}{v}}}\right]\right\}, \\
-\infty < x, y < \infty, 0 \le z \le b, t > \mathbf{0} \qquad (2)
\end{aligned}
$$

The Sagar/Wexler solution is written (Sagar, 1982; Wexler, 1992; Wang and Wu, 2009),

$$
\begin{aligned}
\frac{C}{C_o} = \frac{x}{8\sqrt{\pi D_x}}\int_0^t exp\left[-\lambda\tau - \frac{(x-v\tau)^2}{4D_x\tau}\right] \\
\times\left[erfc\frac{\left(y-\frac{Y}{2}\right)}{2\sqrt{D_y\tau}} - erfc\frac{\left(y+\frac{Y}{2}\right)}{2\sqrt{D_y\tau}}\right] \\
\times\left[erfc\frac{(z-Z)}{2\sqrt{D_z\tau}} - erfc\frac{(z+Z)}{2\sqrt{D_z\tau}}\right]\frac{d\tau}{\tau^{\frac{3}{2}}} \\
x > 0, -\infty < y < \infty, 0 \le z \le b, t > \mathbf{0} \qquad (3)
\end{aligned}
$$

where τ is a time variable and b is the aquifer thickness (L). Full forms and derivations of the Domenico and Sagar/Wexler solutions can be found in Guyonnet and Neville (2004), West et al. (2007), and Srinivasan et al. (2007). The Sagar/Wexler solution is available in a spreadsheet format in BioscreenAT, which is freely available on the internet (Karanovic et al., 2006).

Ease of Use and Speed

For introductory or intermediate students learning transport modeling, working in a spreadsheet environment simplifies the computing. The Domenico solution can be entered directly into Microsoft Excel, which supports the error function (*erf*) and complimentary error function (*erfc*), and is faster to compute than the Sagar/Wexler solution, since it does not require numerical integration. In spreadsheets, this distinction is important because execution times are notably slower than those of codes compiled outside of spreadsheets. To illustrate the importance of this difference, a direct comparison was made. The Domenico solution was entered into an Excel spreadsheet and the Sagar/Wexler solution was evaluated in Visual Basic, within the Excel environment. Both codes generated two-dimensional (2D) representations of plumes with 21 × 21 grid nodes, and were written to run with a Monte Carlo algorithm. Using a Dell Precision T7500 Workstation with Dual Quad Core Intel Xeon Processors X5560, 2GHz, a 200-realization, 240-point, a two-dimensional plume took 23 hours and 40 minutes

(1420 minutes) to compute using the Sagar/Wexler solution. The same 200-realization, 240-point plume was computed in 0.3 minutes using the Domenico solution.

ACCURACY OF THE DOMENICO SOLUTION

Studies critiquing the Domenico solution all reported errors on the order of 80% or more if certain parameter ranges were exceeded. Srinivasan et al. (2007) showed that the discrepancies arise because the Domenico solution replaces the time variable τ with a constant x/v. As a result, the transverse dispersion process is treated as space dependent and time independent. The result is that the Domenico solution approaches exactness as longitudinal dispersivity approaches zero. Accordingly, the error in the Domenico solution is closely associated with the magnitude of the transverse dispersivity parameters. Thus, the use of large values of dispersivity tends to result in large errors in the solution. If the transverse horizontal and vertical dispersivities are treated as functions of the longitudinal value, as is commonly the practice (Anderson, 1984; Bear and Verruitj, 1987; Wiedermeier et al., 1999; Benekos et al., 2006; Delgado, 2007), maintaining a low longitudinal value is prudent. We found that in simulations similar to the ones discussed in the exercises below, longitudinal dispersivities kept well below approximately 10% of the plume length (defined here as the distance from the source to the C/C_o contour of 0.01), resulted in calculated concentrations along the plume center line that agreed to within 20% of the C_o value (see Supplementary Material; available at: http://dx.doi.org/10.5408/11-230S1). This agreement might vary somewhat in other modeled scenarios. In the simulations presented in the supplemental material for this article, the greatest percent differences along the centerline of the plume were associated with scenarios in which transverse dispersivity was underpredicted by the Domenico solution. Nevertheless, the Domenico solution provides a reasonable picture of the bulk of the plume, which is of great value for instruction.

Are Large Dispersivity Values Reasonable?

The fitting of models to field data commonly relies on the identification and quantification of poorly constrained parameters, such as dispersivity or pseudo-first-order rate constants. The Domenico solution returns predicted plume concentrations similar to those of the Sagar/Wexler solution for conditions typical of low dispersion in sandy aquifers (Srinivasan et al., 2007). Since dispersion is expected to be low in these settings (Freyberg, 1986; LeBlanc et al., 1991), use of the Domenico solution is justified for these cases. This justification, discussed in more detail below, is a useful one to bring to the attention of students since it highlights a basic characteristic of dispersion, that is, it is fundamentally a weak process although it may be enhanced by various factors such as aquifer heterogeneity, sorption, physical/chemical non-equilibrium processes, and transient flow. This, coupled with its ease of programming and use, make it eminently useful in the classroom.

In a review of data from 59 field sites, Gelhar et al. (1992) observed an increase in dispersivity with the scale of measurement. The largest high-reliability longitudinal dispersivity value Gelhar et al. (1992) found was 4 m for a plume length of 250 m. Schulze-Makuch (2005) extended the Gelhar et al. (1992) data set to include results from 109 studies. In that work, the longest plume with highly reliable data was in fractured dolomite, and was 597 m long, with a longitudinal dispersivity of 3.7 m (Schulze-Makuch, 2005). Transverse dispersivity values are commonly assumed to be about a tenth (horizontal transverse, α_y) to a hundredth (vertical transverse, α_z) of the longitudinal dispersity, α_x (Anderson, 1984; Wiedermeier *et al*. 1999). On the basis of this prior science, it can be argued that the use of longitudinal dispersivity values in excess of 5–10 m for plumes less than 0.5 km in length is questionable, particularly where granular aquifers are concerned. In addition, reasonable transverse dispersivities are probably less than 1 m. The use of larger values of dispersivity suggests conceptual errors or compromises by the model users. Under these conditions, the usefulness of any analytical solution should be considered provisional. If the answer to the question posed in this section's header is "no," then the Domenico solution can be used with reasonable expectations of accuracy, particularly for bulk plume behavior.

EXERCISES BASED ON THE DOMENICO SOLUTION

The following exercises have been used in whole or in part in the graduate level Contaminant Transport class at the University of Kansas. The assignments were available online along with video files that showed the basic steps involved in creating the Domenico spreadsheet. The use of videos was found to greatly reduce the time students spent debugging their programs, and are recommended to any who adopt these exercises for class use.

Exercise 1. The Error Function and Complimentary Error Function

Most students new to the transport equation will be unfamiliar with the properties of the error function (*erf)* and complimentary error function (*erfc*). The error function is closely related to the cumulative normal distribution function, which conceptually ties the transport equation—in particular the dispersed edges of a plume—to probability calculations. In essence, dispersion is treated as the result of random movement of solute molecules in the same sense as is diffusion in Fick's Law. The two functions *erf* and *erfc* are formally defined as follows:

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \tag{4}$$

$$erfc(x) = 1 - \text{erf}(x) \tag{5}$$

These equations cannot be solved exactly. As a result various estimation methods have been developed. Excel supports these functions, but their accuracy should be assessed before using the spreadsheet in transport calculations, Seven different approximations of the *erf* function are presented in Table I, and are compared to the Excel *erf(x)* approximation in the first of the exercises described for classroom use below.

In our experience, students are rarely familiar with the properties of the error and complimentary error functions, and their approximations. Moreover, they can benefit from a

TABLE I: Summary of *erf(x)* approximations for comparison in the exercise.

erf(x) Approximation	Label; Sources
$erf(x) = \frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n+1}}{n!(2n+1)} \ldots for\ x \leq 3.4$ $erf(x) = 1 - \frac{e^{-x^2}}{x\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{1}{2nx^{2n}(2n-1)} \ldots for\ 14 > x > 3.4$ $erf(x) = 1 \ldots for\ x > 14$	**Series;** Abramowitz and Stegun (1966); High range series adapted from code by E.A. Sudicky
if $x \geq 0$ $erf(x) = 1 - A$ if $x < 0$ $erf(x) = -1 + A$ $A = T \times exp(-\|x\|^2 - 1.26551223 + T(1.00002368 + T(0.37409196 + B)))$ $T = \frac{1}{1+0.5*\|x\|}T$ $B = T(0.09678418 + T(-0.18628806 + T(0.27886807 + C)))$ $C = T(-1.13520398 + T(1.48851587 + T(-0.82215223 + T(0.17087277))))$	**Press;** Press et al. (1992)
$erf(x) \approx \left[1 - \exp\left(x^2\frac{\frac{4}{\pi}+ax^2}{1+ax^2}\right)\right]^{\frac{1}{2}}$; a = 0.140; a = 0.147	**Winitzki;** Winitzki (2003); Winitzki (2008)
$erf(x) = 1 - (1 + 0.278393x + 0.230389x^2 + 0.000972x^3 + 0.078108x^4)^4$	**Abramowitz4;** Abramowitz and Stegun (1966)
$erf(x) = 1 - (0.254829592G + (-0.284496736)G^2 + 1.421413741G^3 + (-1.453152027)G^4 + 1.061405429G^5)e^{(-x^2)}$ $G = \frac{1}{(1+0.3275911*x)}$	**Abramowitz6;** Abramowitz and Stegan (1966)
$erf(x) = 1 - e^{\left(-\frac{16*x^2}{23}-\frac{2}{\sqrt{\pi}}x\right)}$	**Lether1;** Lether (1993)
$erf(x) = 1 - w_1 e^{\left(-(a_1x^2)-b_1x\right)} - w_2 e^{\left(-(a_1x^2)-b_2x\right)}$ $a_1 = 0.9069444$, $w_1 = 0.7897872$, $b_1 = 0.7499586$, $w_2 = 0.2102128$, $b_2 = 2.5501373$	**Lether2;** Lether (1993)

lesson in validating a particular approximation, in this case the one used by Excel.

Assignment Suggestions

1. Students can use a prepared spreadsheet in erfCompare.xlms file (available online at: http://dx.doi.org/10.5408/11-230.s2), in which each of these approximations has been programmed as an internal function. Assuming the series approximation is the most accurate, a series of spreadsheet columns with differences between the series and other approximations (*other–series)* can be calculated. The plotted results can then be examined to determine which of the approximations is most accurate (Fig. 1).
2. Using the simplified version of the Ogata Banks transport equation given by Domenico and Schwartz (1990, p. 640),

$$\frac{C}{C_o} = \frac{1}{2}\left(1 - erf\left(\frac{(R_f x - vt)}{2\sqrt{\alpha_x vtR_f}}\right)\right) \quad (6)$$

where R_f is the retardation effect. The effect of inaccuracies in the estimated *erf(x)* values can be examined. In most cases (the Winitzki approximation excepted) the estimations are reasonable for predicting concentrations as low as 1×10^{-4} of the input concentration, C_o (Fig. 2). However, it might be noted that drinking water limits for common organic contaminants may be much less than 1×10^{-4} of solubilities. For example, trichloroethene has a reported solubility on the order of 1400 mg/L and a drinking water objective on the order of 1×10^{-2} mg/L, amounting to a difference of five orders of magnitude. Therefore, calculations for contaminant transport may require estimates of *erf(x)* from the series expansion routine, the Press algorithm, or the Abramowitz6 algorithm. Conveniently, the Excel 2010 estimates of *erf(x)* are among the most accurate tested here.

It may also be worth pointing out that the errors discussed here are purely mathematical, and may be considerably smaller than the errors in any measured data to which they would be compared. This point is explored further in Exercise 3.

Exercise 2. Sensitivity Analysis

One of the most powerful uses of models is the sensitivity analysis. If the model accounts for all the processes of importance to describe some phenomenon, then the relative importance of the model parameters can be assessed by varying them one at a time in a series of simulations and noting the effect on the outcome. Sensitive parameters exert a large influence when they are changed only slightly; insensitive parameters exert little effect even if they are varied greatly.

To demonstrate a sensitivity analysis to students using a transport model, the Domenico solution is helpful. In this example, the solution will be solved in 2D. To make the Domenico solution behave as a 2D model, it is only

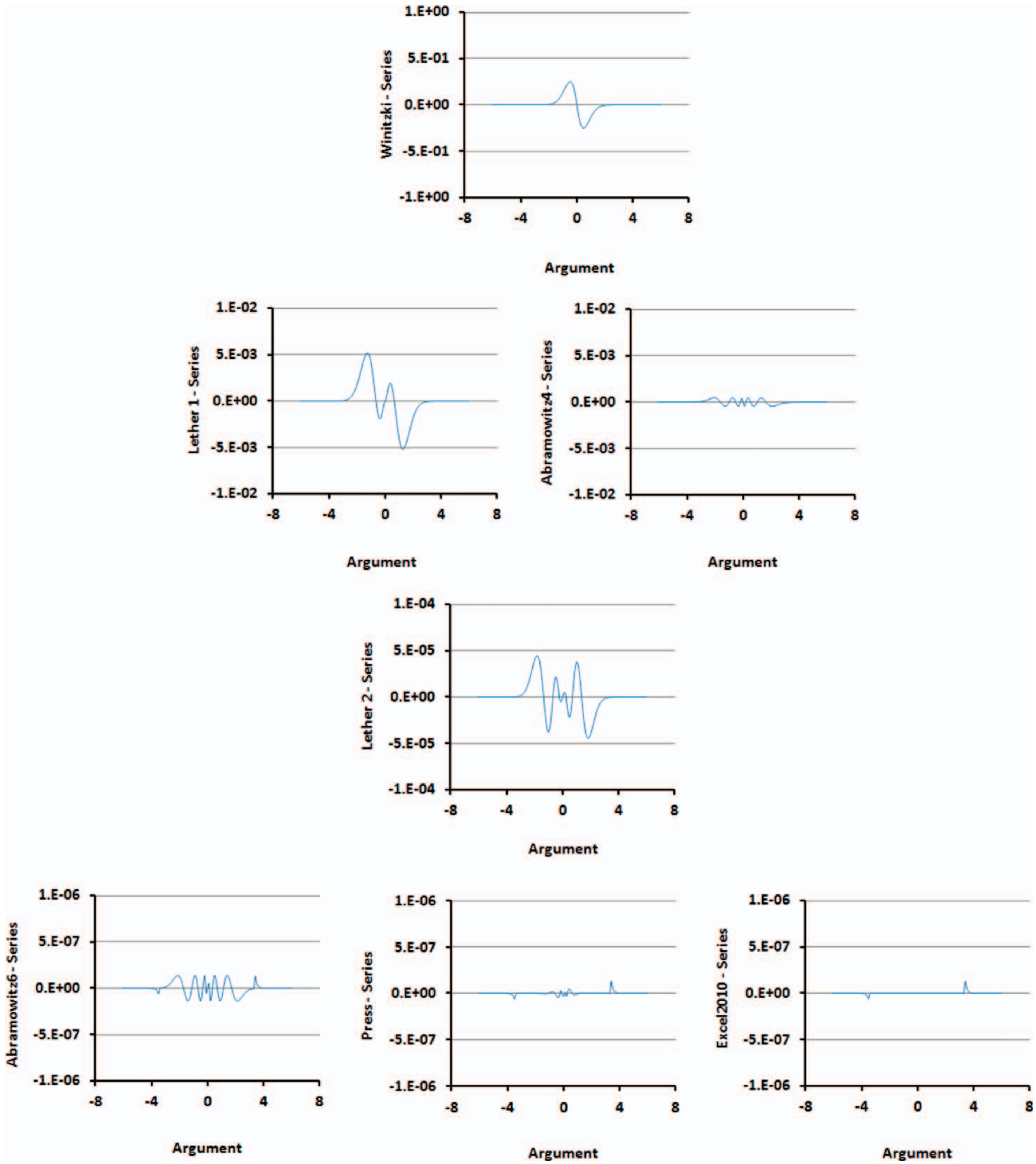


FIGURE 1: Differences between the *erf(x)* estimations and the series expansion (first entry in Table I). The *y*-axis scales decrease by 2 orders of magnitude with each row of graphs down from the top of the figure. The most accurate estimations are therefore from the algorithms associated with the bottom row.

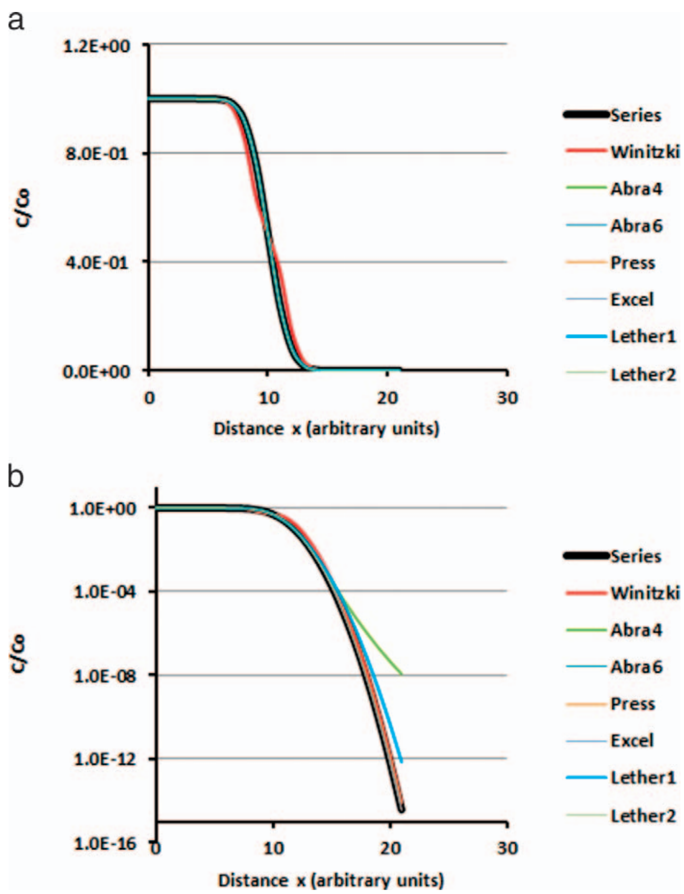


FIGURE 2: Effect of *erf(x)* estimation errors on calculated contaminant concentrations. (a) 1D profile plotted on arithmetic scales showing that the Winitzki equation introduces visible error for $1 > C/C_o > 0$. (b) 1D profile plotted on a semilogarithmic scale showing that at low concentrations the Abramowitz 4 and Lether 1 equations are the most likely to be problematic.

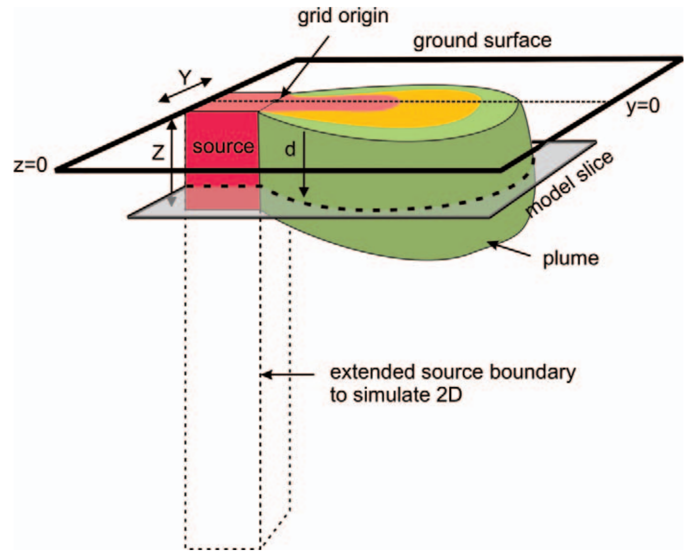


FIGURE 3: Schematic diagram of plume modeled with the Domenico solution (see Assessment of the Domenico Solution section for boundary details). *Y* and *Z* define the source dimensions, *d* the depth to the modeled slice. To ensure that the plume represented in the slice is unaffected by dispersion in the *Z* direction (i.e., if a 2D horizontal plume is modeled), the *Z* value can be made arbitrarily large.

necessary to ensure that the vertical dispersion is not "felt" by the modeled slice (Fig. 3). This is achieved by placing the bottom of the source well below the depth of the slice, that is, choose an arbitrarily large value for Z.

To implement the Domenico solution in a spreadsheet, a conceptually simple approach is to handle each term in the equation separately. For example, Eq. 2 could be rewritten:

$$\frac{C}{C_o} = \frac{1}{8}(Term_1)(Term_2)[Term_3 - Term_4][Term_5 - Term_6] \quad (7)$$

where $Term_1$ is the exponential, $Term_2$ is the *erfc*, and *Terms* 3 to 6 are the respective *erf* terms. Each term is therefore assigned an area of the worksheet, n rows down by m columns across (term areas). The size of n and m depends on the size of the modeled domain and the degree of detail desired. The middle row and leftmost column in each term area is designated the origin (e.g., $x = 1X10^{-6}$ m, $y = 0$). Note that some terms in the Domenico solution involve division by x, so avoid setting $x = 0$. The term areas can be placed in consecutive rows down the worksheet, with the top area reserved for the assembly of the terms into the final equation (Eq. 7; Fig. 4).

An input table is easily created at the top of the worksheet, and if the cells are named in a fashion similar to the designations in Eq. 2, the various terms can be quickly and easily typed into the term areas (note that only the top left cell in each area needs be typed) (Fig. 5). The formulas can be copied to the remaining cells.

The model slice can be visualized by plotting the final term area (Eq. 7) as a surface. The x-axis labels appear on the surface plot automatically but to show the y-axis labels, each row in the term area (called "series" in the Excel environment) must be named. If the naming is done by referencing cells showing the y-distances from the origin of each series (cells A41–A61 in Fig. 4), the y-axis is automatically scaled according to the domain size.

Assignment Suggestion

1. Using the input given in Figure 5 as a base case, change the parameters indicated in the rows of Table II to perform 16 simulations. The relative importance of each parameter to the plume extent and shape, as well as the maximum concentrations in the domain, can be assessed.
2. Comparing the concentrations down the center of the plume in the Domenico solution with those generated from the one-dimensional solution (Eq. 6) gives students an appreciation for the effects and advantages of modeling in 3D.

Exercise 3. Monte Carlo Analysis

Monte Carlo simulations are useful for estimating the propagation of uncertainty through complex equations. Ranges and probabilities are assigned to the input param-

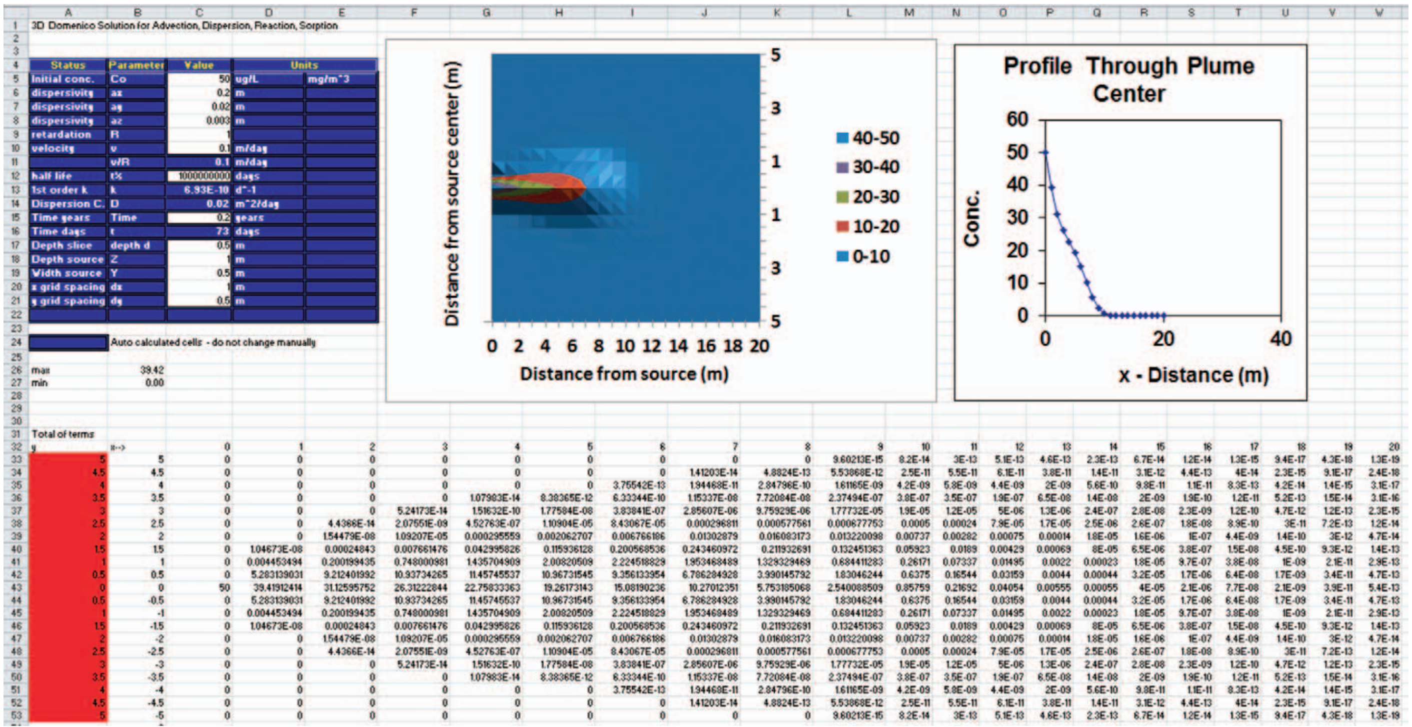
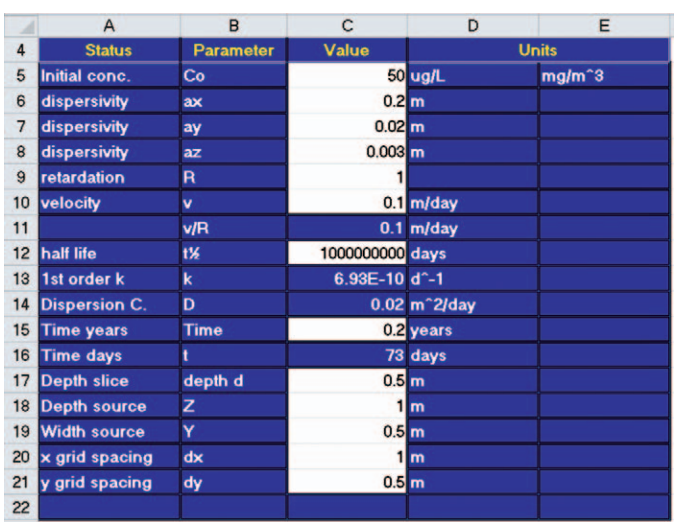


FIGURE 4: Example of input area (upper left), plotted plume slice (upper right), and term area for the equation assembly (bottom, from Eq. 6 in text). Altogether six term areas are present in the worksheet, one corresponding to each term as defined in Eq. 6.

eters and the parameters are then randomly varied to produce many simulations (called "realizations") of plumes. The range and probability of concentrations at any point in the domain can be determined by analyzing the collection of realizations. To obtain a statistically meaningful analysis, many realizations are required. Ideally the number of realizations should exceed 1,000, although for illustrative purposes, 200 realizations is convenient and conveys the essential lessons.



	A	B	C	D	E
4	Status	Parameter	Value	Units	
5	Initial conc.	Co	50	ug/L	mg/m^3
6	dispersivity	ax	0.2	m	
7	dispersivity	ay	0.02	m	
8	dispersivity	az	0.003	m	
9	retardation	R	1		
10	velocity	v	0.1	m/day	
11		v/R	0.1	m/day	
12	half life	t½	1000000000	days	
13	1st order k	k	6.93E-10	d^-1	
14	Dispersion C.	D	0.02	m^2/day	
15	Time years	Time	0.2	years	
16	Time days	t	73	days	
17	Depth slice	depth d	0.5	m	
18	Depth source	Z	1	m	
19	Width source	Y	0.5	m	
20	x grid spacing	dx	1	m	
21	y grid spacing	dy	0.5	m	
22					

FIGURE 5: Example of input screen. Data entry occurs in the white cells. Cells with darker background are not changed and may contain formulas.

Assignment Suggestions

1. To investigate the usefulness of the Domenico solution along the plume centerline, the example from West et al. (2007: Table 2, p. 132) was calculated using the Sagar/Wexler solution, assuming a longitudinal dispersivity of 8 m, a magnitude twice the largest high reliability estimate of 4 m, and a near worst case scenario for a plume several hundred meters in length. The example was then recalculated 200 times using the Domenico solution programmed in Excel with a Monte Carlo algorithm written in Visual Basic (see worksheet in DomenicoFullMonteCarlo file available online at: http://dx.doi.org/10.5408/11-230.s3). Lognormal distributions with mean longitudinal dispersivities of 1 m and 8 m were assumed. A 95% confidence range of 3 m to 21 m—slightly narrower than that proposed by McNab and Dooher (1998)—was assumed for the 8 m longitudinal dispersivity simulation, corresponding to an approximate standard error of ±0.4 in natural log units (~ ±3 m as dispersivity), which was used in both simulations. Other input parameters were taken from West et al. (2007). The Sagar/Wexler lines in Figure 6 do not track through the middle of the Domenico points. This reflects slight asymmetry in the concentration distribution calculated from the Monte Carlo analysis and error in the form of bias in the Domenico solution, which is consistent with the findings of West et al. (2007), and especially noticeable in Figure 6B. However, the simulation shows that once the uncertainty in dispersivity is taken into account, the Sagar/Wexler solution falls within the range calculated by the Domenico model for the plume centerline (Fig. 6A). So, the differences in α_x needed to produce similar plumes via the two solutions are statistically insignificant in this example.

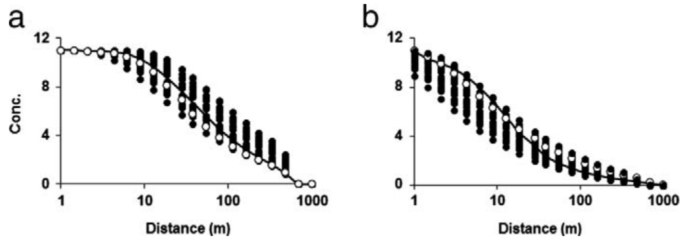


FIGURE 6: Domenico (1987) Monte Carlo solutions (circles) and Sagar (1982)/Wexler solution (line) compared for a 5-year simulation assuming a longitudinal dispersivity (α_x) of (a) 1 m and (b) 8 m, $\alpha_y = \alpha_x/10$ and $\alpha_z = \alpha_x/1000$. Open circles show the Domenico solution with a longitudinal dispersivity of (a) 1 m and (b) 8 m. Note the distance axis is on a log scale. Concentrations are in arbitrary units. Results of 20 realizations, representing the range of outcomes, are shown.

In practical terms, important decisions should not be made on the basis of either solution using only one of these dispersivity values. However, to gain preliminary insights into plume behavior, either solution can be useful if low values of dispersivity are considered.

ASSESSMENT OF LEARNING

To evaluate the effectiveness of the Domenico solution (and spreadsheet exercises in general) in promoting the learning of transport concepts, students in a graduate Contaminant Transport class (n = 11) were surveyed after taking a course that used them in assignments (Fig. 7). The class included both PhD and MS students, with the latter being in the majority. Students were required to have taken an introductory course in hydrogeology, as well as calculus previously. A prerequisite of differential equations was also suggested but not strictly enforced. At the conclusion of the course, an independent assessment of students' abilities to use these tools and skills in projects was also undertaken through the evaluation of an assigned project (Figs. 8 and 9).

The seven-question survey (Fig. 7) showed that students felt their knowledge of the subject was poor at the outset of the course, but was greatly improved by the end. The first two questions asked students to rate their knowledge of transport processes in general, and modeling in particular at the outset of the course. The next two questions asked students to rate their ability to solve an analytical problem with a spreadsheet, and to rate the degree to which their understanding of transport processes was improved through modeling with the Domenico solution. Students were then asked, based on their prior experiences with commercial software packages (transport and others), to rate the degree to which their understanding might have been improved if the assignments had utilized preprogrammed commercial software packages instead of the Domenico solution. That is, did the students feel the coding components of the assignments enhanced or diminished their learning? Finally, students were asked to rate the value of the skills they had learned and the improvement in their understanding of contaminant transport. The responses suggest that, in the students' views, the spreadsheet exercises were highly beneficial to learning, and the Domenico solution was

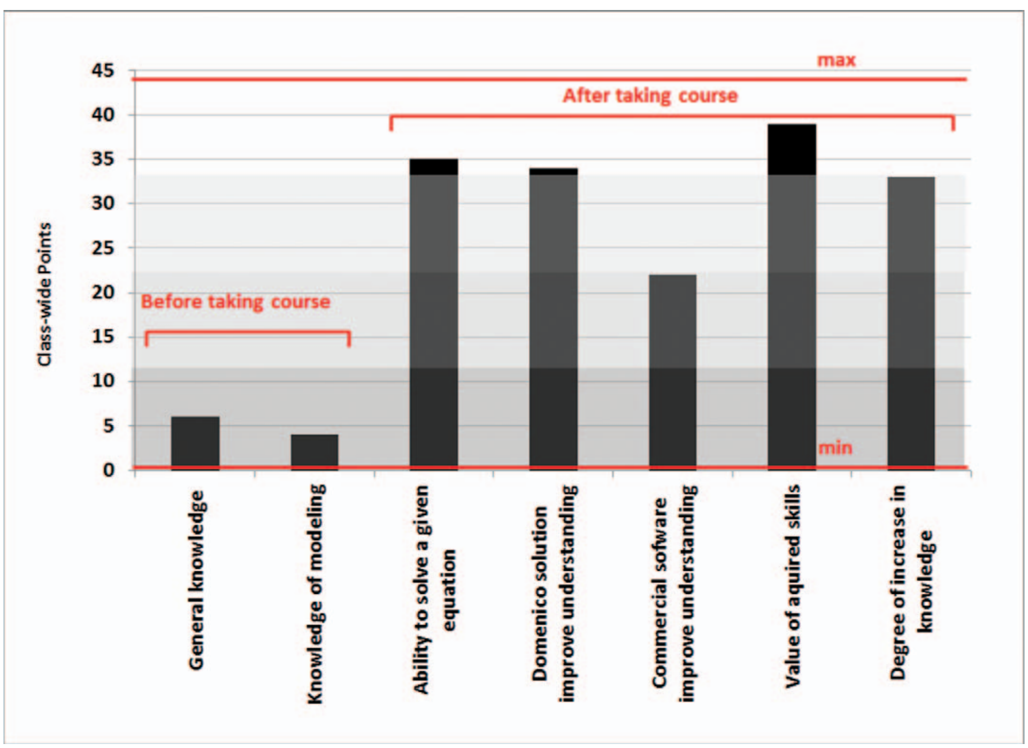


FIGURE 7: Histogram of total class scores for responses to questions concerning prior knowledge and learning successes. Each question was scored 0 to 4. Answers dominated by scores in the bottom 25% of the maximum possible score plot in the dark gray area near the bottom of the chart. Answers scoring in the upper 25% plot in the white area at the top of the chart.

TABLE II: Simulations to be performed. After each simulation, return the input to the settings given in Figure 2 before making the changes for the next simulation.

Simulation	ax	ay	v	R	max C
1	0.05				
2	0.5				
3	5				
4	50				
5		0.005			
6		0.05			
7		0.5			
8		5			
9			0.05		
10			0.01		
11			0.5		
12			2.0		
13				2	
14				10	
15				5	
16				20	

particularly helpful. The students were also very enthusiastic about the quantitative analysis skills they developed in performing the exercises.

The student projects, due at the end of the course, were based on topics or case studies chosen by the students themselves for analysis using the techniques developed in the course. Topics were varied, such as the calculation of degradation sequences in flowing systems, the effects of density flow on diffusion in porous media columns, and phase 1 risk assessment modeling. The results were presented formally to the entire class. Learning was assessed with a rubric developed specifically for the purpose (Fig. 8).

The results of the rubric analysis (Fig. 9) revealed trends very consistent with the results of the student survey (Fig. 7). Students' use of the models were judged to be within 25% of the maximum possible score, similar in magnitude to the students' assessments of themselves. Demonstrated understanding of concepts was slightly weaker, and similar to the level of research skill demonstrated. Presentation quality, which relied strongly on the graphics output by the spreadsheet programs, was very strong.

These results show that exercises, like the ones presented here, can be effective tools for the teaching of pollutant transport in groundwater as well as introductory modeling. Success is indicated both in terms of instructor assessment and student opinion of the instructional methods.

	1	2	3	4	5
Concepts	Poor grasp of concepts and/or scope of talk too limited	Signs that concepts are understood but little scope, weak present.	Good grasp of concepts, good present., scope could be broader	Above expected grasp of concepts, well explained	Superior grasp of concepts, present. and scope
Model	Errors in execution, badly conceived scenario, no originality	Good idea, weak originality, model unsuccessful	Good idea, some originality, minor or no model problems	Good idea, some originality, well executed	Excellent idea, original use of skills, model performed well
Research	No supporting research included	Research limited to class material	Research included one relevant outside paper	Research drew on outside material effectively	Research from outside sources drove modeling approach
Presentation	Difficult to hear, poor slides, distractions, poorly timed	Audible with no distractions but slides poor and timing bad	Audible, no distractions, good timing but slides could be improved	Engaging presentation with minor improvements needed	Professional level presentation, no improvements needed

FIGURE 8: Rubric used to evaluate student learning as demonstrated by the project presentation (see text). Note "present." is short for "presentation" in the table.

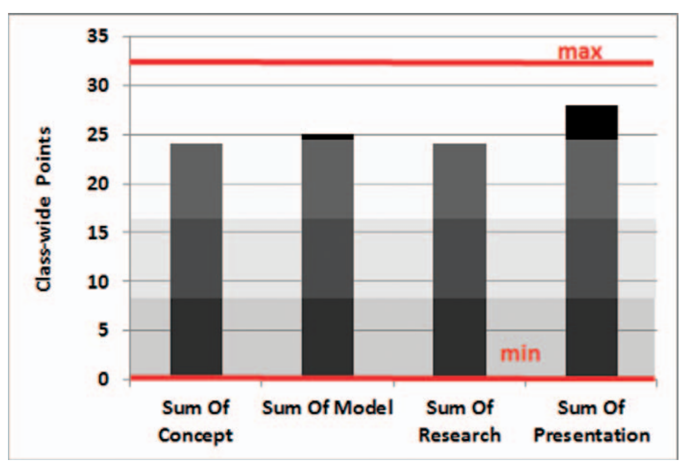


FIGURE 9: Histogram of the instructor assessment of student presentations, based on the four points of interest listed in the rubric (Fig. 8): grasp of concepts, modeling proficiency, supporting research, and presentation quality. Sums of class-wide points are given.

CONCLUSIONS

The Domenico solution is a heuristically derived equation that closely approximates rigorous solutions to the advection dispersion equation under conditions that are representative of real world plumes. The equation has been criticized because it is only an approximation, but for instructional purposes it can provide students with useful insights. The equation is relatively easy to input into an Excel spreadsheet, gives students experience creating a model from scratch, executes quickly, and can be used to illustrate the use of sensitivity analyses, effects of spatial dimensions, and the application of Monte Carlo analysis. Students rated the Domenico solution, and spreadsheet-based exercises in general, highly beneficial in improving their understanding of modeling and transport concepts. The student opinions were consistent with an independent instructor evaluation of projects that utilized the spreadsheet skill set.

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