Analysis of a Dirty Motor Pool

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A topic of enduring concern to military operators and logisticians is the environmental signature left by both field and garrison operations.

This paper details one of the scenarios which we use in our engineering math course to excite and motivate future environmental engineers about uses of mathematics in their discipline. This scenario illustrates the use of vector calculus, partial differential equations (PDE's), and numerical methods, along with a computer algebra system (MathCad) and spreadsheet (Excel), in modeling the advection and diffusion of an oil spill.

Working through this scenario exercises the following mathematical skills:

- Parameterization of space curves, using vector differential operators, and using the vector integral theorems
- Modeling using PDE's
- Solving the diffusion equation via separation of variables
- Making engineering value judgments (such as how much seepage is "appreciable", vs. nonzero)
- When and how to use the dominant eigenmode as a long-term approximation
- Refining a model to incorporate new effects
- Numerically (via finite differences and a spreadsheet) solving more complex variants of the diffusion equation
- Graphing solution curves and drawing inferences

Scenario

You are a Battalion Executive Officer stationed in Korea. Among your many duties, you are in charge of vehicle maintenance and motor pool operations for the battalion. The Assistant Division Commander for Support (ADC(S)) is flying over your battalion motor pool area one morning, and happens to notice some ground discoloration near the Brigade POL (Petroleum, Oils, and Lubricants) Tank Farm, for which you have primary responsibility. He later calls your commander and you and tells you to investigate. Your initial check shows that one of the fuel storage tanks has started to leak at a seam. It is a large-area ground oil spill with continued leakage (maintaining the surface at a constant level of contaminant concentration). The contamination is being advected by surface runoff and is also diffusing downward toward bedrock level. The Facility Engineers estimate that it will take 72 hours to repair the pipe and stop the leak. The local civilian Environmental Officer immediately calls and demands to know where runoff will carry the contamination, to what depth contaminated soil will have to be excavated after the leak has been stopped, and what the effect would be on the spread of contaminant if the weather is rainy over the next week.

Tracking Avective Processes and Runoff

You decide to analyze the quickest acting process first: runoff. A quick survey of the terrain shows that the major runoff for the contaminant appears to be the stream flowing from near the spill (point A on the map below) toward point B, near the neighboring town. The vertical grid lines are 1000m apart, the horizontal grid lines are 750 m apart, and contour lines are at elevations as marked on the map.

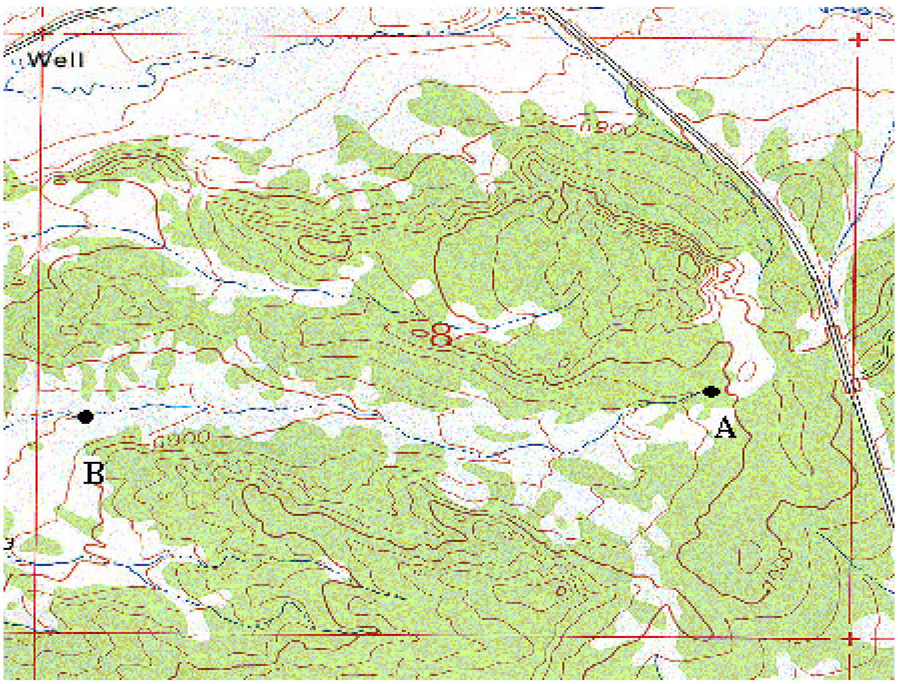

Figure 1: Path of stream from at Point A to B.

Example 1: Mathematically model the path in order to determine the flow of the stream.

Solution: We begin by using Mathcad to plot a model the stream. We write a parametric vector function for the position of a marker particle in the stream as it moves from A to B. A possible parameterization of the streambed is the parametric equation $\boldsymbol{r}(t) = (e^{2t} \sin 7t + \sin 15t)\,\boldsymbol{i} + 800t\,\boldsymbol{j} + 130t\,\boldsymbol{k}, \quad 0 \le t \le 1$ (where t is measured in seconds and x, y, z are measured in meters). As graphically illustrated in Figure 2, this yields a good approximation to the path of the stream.

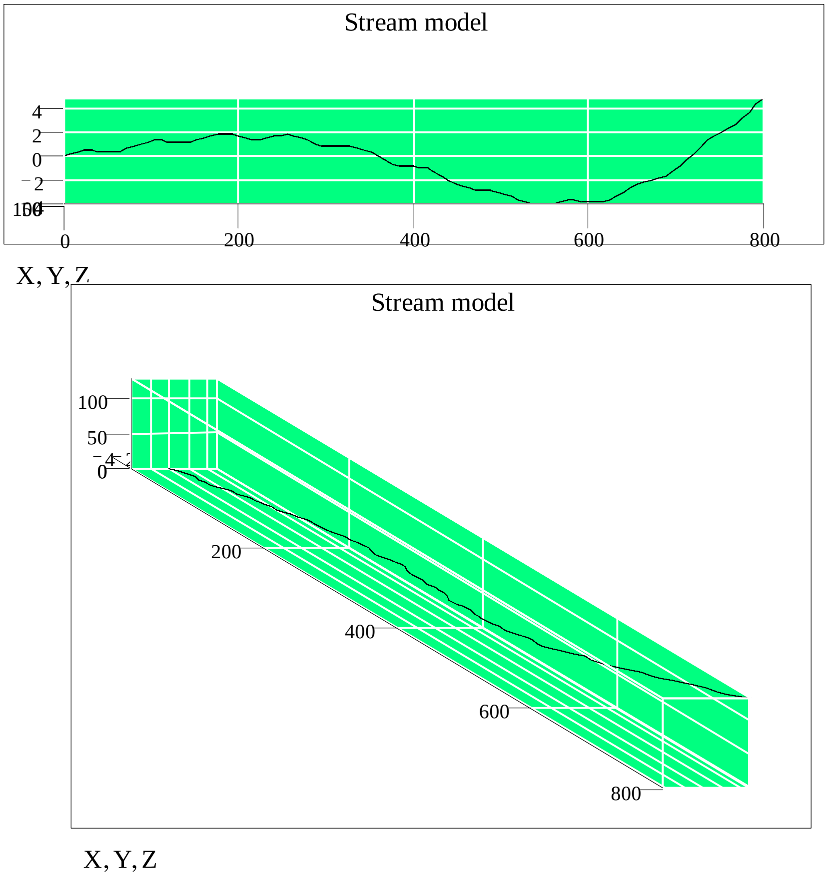

Figure 2: Parameterized representation of the Advecting Stream

Example 2: Given the above position function of the stream, with A at $t=1$ and B at $t=0$, you measure and approximate that the water's velocity field is in fact $\boldsymbol{v} = 0.1\boldsymbol{i} - 0.2\boldsymbol{j} - 0.1\boldsymbol{k}$. Find the flow of water (as defined in Finney/Thomas, Revised Printing, p.952) moving in the one-dimensional model of the stream between A and B. Describe what this means physically, including the sign of the result.

Solution: The flow of the advecting stream is calculated via the line integral $\int_C \boldsymbol{v} \cdot d\boldsymbol{r}$ for the given velocity field, yielding:

$$r \int_C \boldsymbol{v} \cdot d\boldsymbol{r} = r \int_0^1 \boldsymbol{v}(t) \cdot \boldsymbol{r}'(t)\, dt = -215.6\, m/s.$$

This is a combined measure that indicates both how far and how fast the fluid is moving. It is negative, which means that the net flow velocity is in the direction from A toward B. The magnitude, obtained by dividing the total flow by the length of the stream, is of about the correct order, as the Colorado River has a flow of from 300 to 1000 m^3/s.

We now seek to determine the effect of vorticity on contaminant monitoring equipment placed in bore holes that we dig at several specified locations along the length of the stream. Several boreholes have been dug near the spill site and instruments placed in the wells to obtain data on the effect of the spill. (See figure below). Each hole is cylindrically shaped, 2 meters deep and 20 cm in diameter. In one of the holes, the velocity field is measured to be $\boldsymbol{v} = x\boldsymbol{i} + y\boldsymbol{j} - 3z\boldsymbol{k}$ m/s (with origin centered at the bottom of the hole).

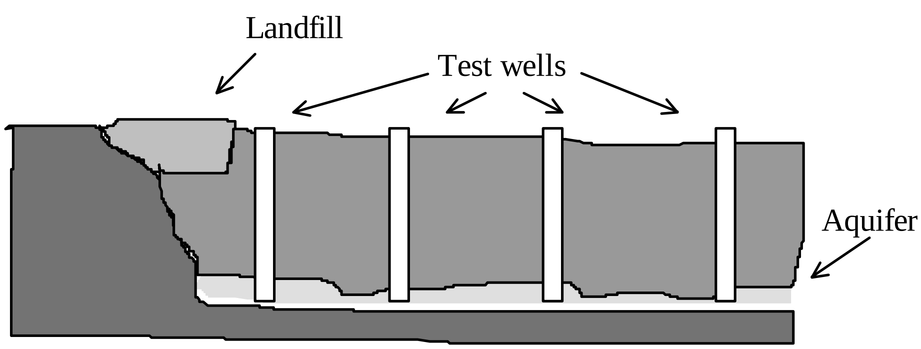

Figure 3: Bore holes for contaminant measuring equipment.

Example 3: At what rate is water entering the hole from above?

Solution: The flux of water into the hole is given by

$$\iint_A \boldsymbol{v} \cdot \boldsymbol{n}\, dA = \iint_A < x, y, -3z > \cdot \boldsymbol{k}\, dA = \iint_A -3z\, dA = -3 \cdot 2 \iint_A dA = -6A = -0.1885\, m^3/s\ .$$

The sign is negative since net flux is opposite in direction to the outward normal vector; i.e., net flux is downward through the upper surface.

Example 4: Are there any sources or sinks in the interior of the hole? Describe.

Solution: From the velocity field of the fluid in the borehole, we calculate that the divergence at all points is $\nabla \cdot \boldsymbol{v} = 1 + 1 - 3 = -1$ per sec. Since the divergence is negative at all points, this indicates that there is a sink at every point in the hole. This might occur if the density of the fluid decreased after it entered the hole, perhaps due to warming by the equipment in the hole.

Example 5: At what rate is water entering the hole from all sides (including the porous sides and bottom, as well as the top)?

Solution: The total flux of fluid into the hole can be calculated by transforming the closed surface integral $\oiint_s \boldsymbol{v} \cdot \boldsymbol{n} ds$ into the volume integral $\iiint_V \nabla \cdot \boldsymbol{v} dV$ via Stoke's Theorem, yielding $\iiint_V -1 dV = -1 \cdot V$; this gives a net flux into the hole of $-.06275 m^3 / s$.

In another of the test wells, ground water rotates around the center of the hole (within the plane z = 1) with velocity $\boldsymbol{v} = w(y\boldsymbol{i} - x\boldsymbol{j})$, where w, the angular velocity, is 0.25 rad/s. If the circulation in the well exceeds 15 m^2/s, the data collected by instruments in the well will be corrupted.

Example 6: Will the empirical results obtained from that hole be valid?

Solution: The flow circulation around the midpoint plane of the cylindrical hole can be found by transforming the line integral $\oint_C \boldsymbol{v} \cdot d\boldsymbol{r}$ into the double integral $\iint_A \nabla \times \boldsymbol{v} dV$ via Gauss' Theorem. This yields:

$$\iint_A < 0,0,-2w > \cdot \boldsymbol{k} dA = -2wA = -0.0157 \text{ m}^2\text{/s}.$$

The circulation is much less than the critical value of the equipment; therefore, collected data will be reliable.

Calculating Downward Diffusion

You now turn your attention to the contamination of the ground underneath the spill due to diffusion. You begin with the following assumptions:

- The spill is uniform over an area large enough such that there is diffusion only in the vertical direction.
- The soil is homogeneous with a diffusion rate of 0.3 ft^2/hr.
- There is no advection.
- The leak is such that it maintains a constant concentration of 5000 g/ft^3 over the surface.

- There is bedrock beginning at a depth of 20 ft which is impervious to fuel.

Example 7: Determine how much soil must be excavated.

Solution: We begin by modeling the contaminant diffusion by the equation $\partial u / \partial t = 0.3 \partial^2 u / \partial t^2$, which we will hereafter abbreviate as $u_t = 0.3 u_{xx}$, where u is the local concentration of contaminant, along with boundary conditions $u(0,t) = 5000$ (constant concentration in the spill area), $u_x(20,t) = 0$ (impermeable at the permafrost level), and initial condition $u(x,0) = 0$ (initially clean). Separation of variables yields the infinite series solution

$$u(x,t) = 5000 - 20000/p \sum_{n=1}^{\infty} 1/2n - 1 \, \mathrm{Sin}((2n-1)px/40)\, \exp(-0.3(2n-1)^2 p^{2t}/40).$$

Plots of contaminant concentration at fixed depths over time and at fixed times as functions of depth are shown in Figure 4.

Solution at Fixed Depths over Time:

$t2 := 0, .1 .. 72$

Solution at Fixed Times as a Function of Depth:

$x2 := 0, 0.1 .. 20$

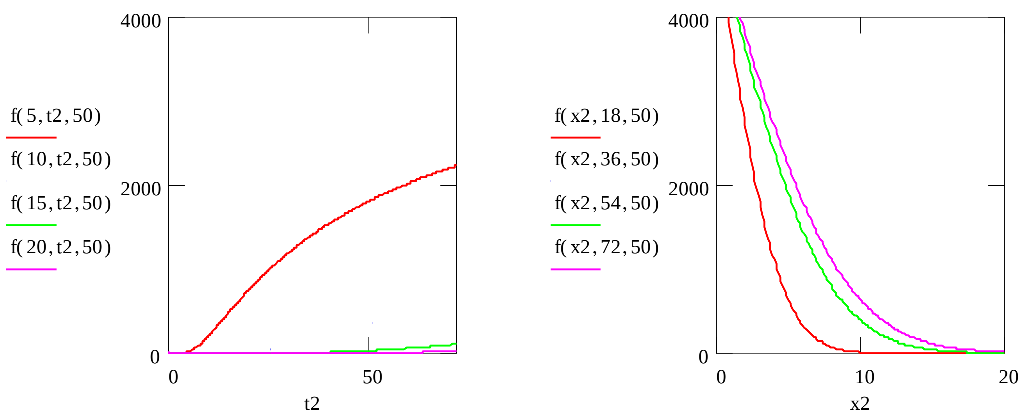

Figure 4: Contaminant concentration at fixed depths and fixed times.

The answer to the question "how much to excavate?" is: it depends on how long you wait and what concentration of contaminant is acceptable. For example, waiting 72 hours means that we will have to excavate to bedrock level (20 ft) if we cannot tolerate a contaminant concentration greater than 500 g/m^3. What level of contaminant concentration is unacceptable? If we are interested only in the physical effects of contamination, then chemistry and physiology can sometimes give us an answer; those disciplines can help us estimate at what level will the contaminant show up as a marginal health hazard in our local drinking water or in the aquifer for the larger community, and that is where the scientist would be inclined to draw the line. However, from a psychological standpoint, local residents may take decades to accept the fact that their homes sit and their children play in the dirt above contaminants, even if the concentration is well below the physiological threshold. Economically, property values may suffer for decades for the same reason. Legally, owners and developers may carry the additional risk of being held liable for random health problems, even if not clearly related to the presence of contaminants. Obviously, the decision as to what constitutes a "tolerable" concentration greatly effects the results to our question, and is as much (usually more) a political decision as it is a scientific one. (An important learning point for engineers!)

In many situations involving diffusion (such as under land fills), environmental engineers are often concerned only with solutions at large times (often on the order of decades), and not with transients over short time scales. We can derive such a simpler long term solution to our situation above by recognizing that higher order modes become increasingly less important over time, yielding (for example) the much simpler two term approximation for the contaminant concentration at long times:

$u(x,t) = 5000 - 20000/p \,\mathrm{Sin}(px/40)\, \exp(-0.3p^2 t/1600)$.

Calculating Downward Diffusion with Advection

We have analyzed the pure diffusion case; now we have to deal with the addition to the model of another physical process; namely, advection of the contaminant downward due to rainfall.

Example 8: Determine whether rainfall will have any effect on our results on the downward diffusion of contaminant.

Solution: Analytic techniques appear harder in this case, so we turn to a numerical method. To predict the differences that would be caused by rainwater advection (downward) if we have rain, we consider a model that incorporates both diffusion and advection: $u_t = 0.3u_{xx} - 0.01u_x$, along with the previous boundary and initial conditions.

We difference the equation using forward first differences in time and centered first and second differences in space, resulting in the algorithm (which we abbreviate as the FTCS algorithm, for forward-time, centered-space):

$$u_{j,k+1} = u_{j,k} + 0.3\,{\Delta t}/{\Delta x^2}\,(u_{j-1,k} - 2u_{j,k} + u_{j-1,k}) - 0.01\,{\Delta t}/{2\Delta x}\,(u_{j+1,k} - u_{j-1,k})\,. \qquad \textbf{(1)}$$

We implement this in a spreadsheet, as demonstrated in the figure below. Spatial grid points are numbered horizontally in dark shade, temporal grid points vertically in dark shade, initial condition horizontally in light shade, boundary conditions vertically in light shade.

t / x	0	2	4	6	8	10	12	14	16	18	20
0	0	0	0	0	0	0	0	0	0	0	0
1	5000	0	0	0	0	0	0	0	0	0	0
2	5000	375	0	0	0	0	0	0	0	0	0
3	5000	693.75	28.125	0	0	0	0	0	0	0	0
4	5000	966.7969	75.9375	2.109375	0	0	0	0	0	0	0
5	5000	1202.473	137.2148	7.488281	0.158203	0	0	0	0	0	0
6	5000	1407.393	207.3797	16.66802	0.696094	0.011865	0	0	0	0	0
7	5000	1586.837	283.0773	29.7735	1.842671	0.062292	0.00089	0	0	0	0
8	5000	1745.043	361.8615	46.67647	3.803955	0.191216	0.005428	6.67E-05	0	0	0
9	5000	1885.426	441.9612	67.09991	6.748438	0.448237	0.01896	0.000464	5.01E-06	0	0
10	5000	2010.759	522.1065	90.68815	10.80228	0.888556	0.049769	0.001817	3.9E-05	3.75E-07	3.75E-07
11	5000	2123.303	601.399	117.0531	16.05019	1.569177	0.109081	0.00528	0.000169	3.28E-06	3.28E-06
12	5000	2224.913	679.2159	145.8038	22.53933	2.545746	0.210803	0.012682	0.00054	1.57E-05	1.57E-05
13	5000	2317.117	755.1373	176.5649	30.28465	3.870144	0.371065	0.02663	0.001412	5.51E-05	5.51E-05
14	5000	2401.185	828.8928	208.9868	39.27458	5.588801	0.607663	0.050571	0.003201	0.000157	0.000157
15	5000	2478.174	900.3217	242.7513	49.47656	7.74165	0.939467	0.088801	0.006526	0.000385	0.000385
16	5000	2548.972	969.3429	277.5735	60.84205	10.3616	1.385831	0.14643	0.012236	0.000846	0.000846
17	5000	2614.327	1035.932	313.2013	73.31088	13.47445	1.966059	0.22932	0.021446	0.0017	0.0017
18	5000	2674.873	1100.107	349.4144	86.81493	17.09906	2.698933	0.343985	0.035556	0.003181	0.003181
19	5000	2731.15	1161.913	386.0214	101.2812	21.24774	3.602321	0.497474	0.05626	0.005609	0.005609

Figure 5: A spreadsheet (Excel) implementation of the finite difference (FTCS) solution.

We can then graphically compare the effects of diffusion alone versus diffusion with convection.

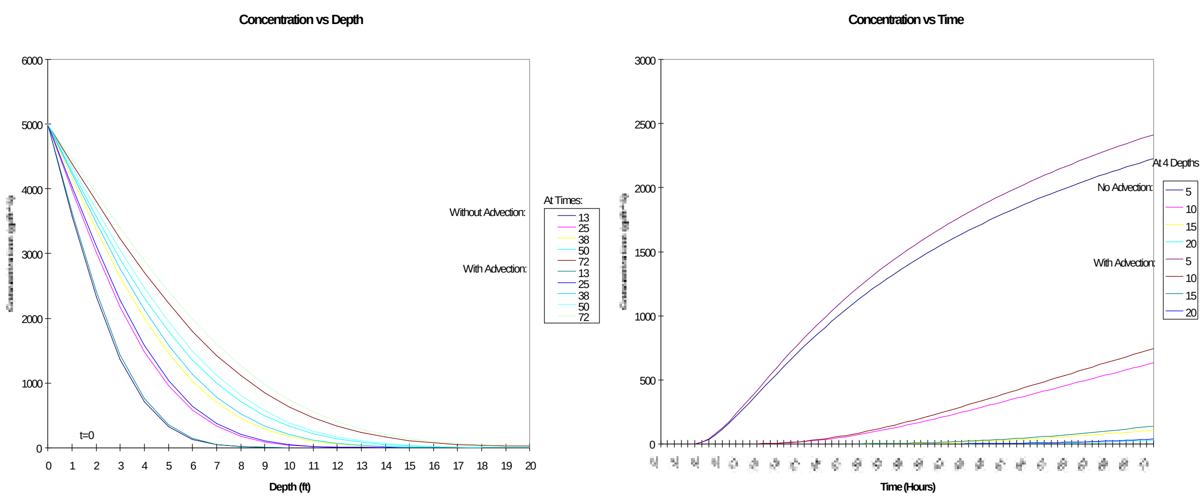

Figure 6: Comparison of diffusive and diffusive-advective solutions.

In this scenario (with an advective coefficient of 0.01), we see that advection due to rainwater only slightly (by about 10%) speeds the downward movement of contaminant.

Extensions

Given the numerical (FTCS) procedure we used in the previous requirement, we are in a position to investigate other issues and complications. Convergence issues are present in both our analytic and numerical solutions; the analytic solution suffers from truncation errors when calculating from the infinite series solution, whereas the numerical solution suffers from the propagation of roundoff errors and possible instability (Figure 7).

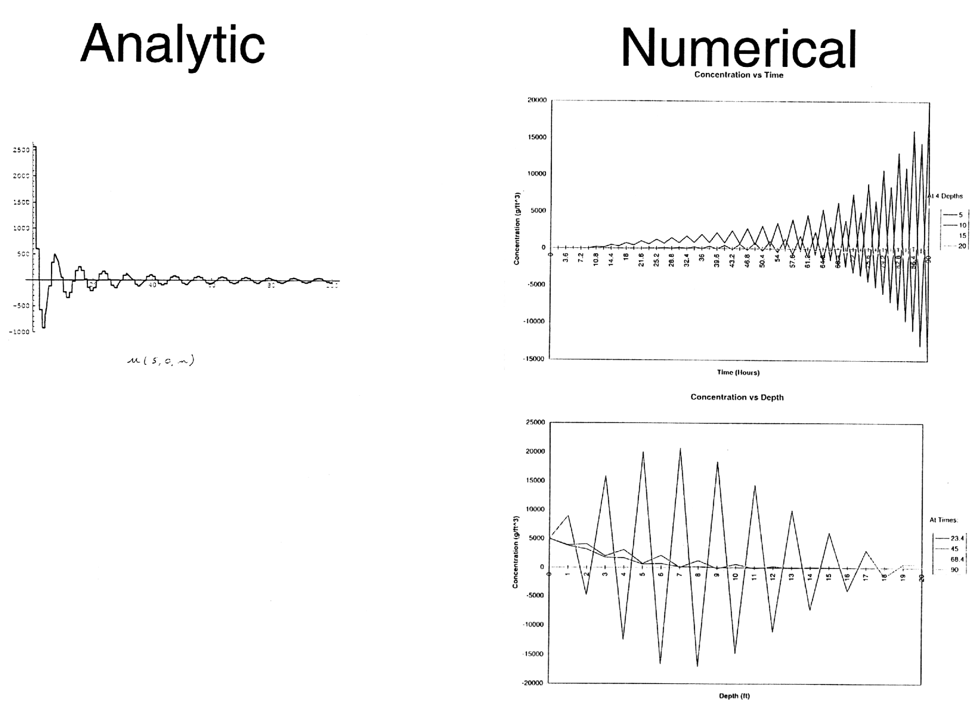

Figure 7: Truncation error (analytic solution) and instability (numerical solution). On the left is plotted the truncation error in the analytic solution vs. number of terms retained in the infinite sum. On the upper right is the numerical solution of Eqn 1 at a given depth as a function of time; note the apparently unbounded temporal error of the unstable solution. At lower right is the numerical solution of Eqn 1 at a given time as a function of depth; note that although the function obeys the boundary conditions, we have oscillations (reaching nonphysical negative values for the concentration) that indicate spatial instability.

Other complications can also be investigated numerically, such as the effect of nonhomogeneous ground porosity (turning the equation into a variable coefficient PDE), the effect of boundaries in a small-area spill, the breakdown of contaminant over time due to chemical reactions, and the effect of slowing or stopping the leak earlier before cleanup can begin (introducing a time dependent boundary condition).

The finite differences and the spreadsheet can be used as above to investigate the introductory combined diffusion-advection scenario. This leads naturally into more realistic, messier groundwater flow problems and more sophisticated numerical codes that are typically used in later hydrogeology and environmental engineering courses.

Exercises

1. Look up Darcy's law (found in most environmental engineering texts, such as references [1] or [2]). Describe how this law can extend the ideas of this project to more general advection problems in atmospheric, reservoir, and water table modeling.

2. In our separation of variables solution for the pure diffusion scenario above, compare the ratio of the first and second terms of the sum when t=0, t=10, t=20, t=30. Repeat for the ratio of the second and third terms. What is the trend? What does this imply about the long term solutions to the diffusion equation?

3. Our separation of variables solution for the pure diffusion scenario expressed the contaminant concentration as a function of depth and time. Instead of plotting curves at constant depth and time, we could instead just plot this equation as a surface; engineers call this a response surface. Describe how we could use the response surface to graphically generate the curves of Figure 4.

4. You are the facility engineer in Berlin. The city of Dresden calls and asks your assistance in making clean up estimates for an old (now unoccupied) Soviet tank company motor pool. The ground has been saturated with POL, and the city government wants to excavate the contaminated soil and replace it with clean fill in order to build low cost housing on the site. The tank company occupied the site for 35 years, and appears to have routinely dumped waste POL during the entire period. Given that the average local diffusivity of the soil is 1.75 m^2/yr, to what depth will the soil need to be excavated?

5. Use the numerical method developed above to rework the pure diffusion scenario. Compare the results numerically (at a few specific points and times) and graphically (at a few times and a few depths). What is the error? How does the difference change when you take more terms in your infinite sum? How does the difference change when you us smaller intervals? Which method do you think is more accurate? Which is faster? Which is more adaptable to harder problems?

6. Starting with our PDE model for diffusion with advection, add a term that might reasonably account for the chemical breakdown of contaminant over time. Solve your new model numerically. How does your new term affect the solution?

7. Look up flow nets and potential flow (found in most environmental engineering or fluids mechanics texts, such as references [1] and [2]). Describe how these extend the ideas of this project to creeping flows in porous soil.

References

[1] Domenico, Patrick A., and Schwartz, Franklin W., *Physical and Chemical Hydrogeology*, 2d Ed., New York: John Wiley & Sons, 1998.

[2] Fetter, Charles W., *Applied Hydrogeology*, 3d Ed., Upper Saddle River, NJ: Prentice Hall, 1988.

[3] Finney, Ross R., and Thomas, George B. Jr., *Calculus (Revised Printing)*, Reading, MA: Addison Wesley, 1991 (p. 952).