FINAL EXAM   University of South Florida

Wed., May 4, 2005   Spring 2005

120 points total   J. A. Cunningham

Instructions:

(1) You may read these instructions, but do not turn the page or begin working until instructed to do so.

(2) Answer all questions in the exam booklet provided, and write your name conspicuously on the exam booklet.

(3) You are allowed two sheets of 8.5-by-11-inch paper with hand-written notes. You may write on both sides of those papers. However, mechanical reproductions (photocopying, laser printing, scanning, faxes, etc.) are not allowed; all notes must be hand-written. A calculator is recommended, but it may not be pre-programmed with formulae from the class.

(4) Time limit: 120 minutes. Stop working when asked. If you continue working after time has been called, you will be penalized at a rate of 1 point per minute.

(5) Show all work and state all assumptions in order to receive maximum credit for your work.

(6) Make sure your answers include units if appropriate. Watch your units!!

(7) This exam contains 5 questions, some with multiple parts. The point value of each question is indicated. The total number of points is 120 — one point per minute, so gauge your time accordingly.

(8) You may read all the information on this side of the page, but do not start working on the exam until instructed to do so.

(9) Use a reasonable number of significant digits when reporting your answers. *You are likely to be graded down* if you report an excessive number of significant digits. In some cases, the problem may indicate the precision to which you should report your answer.

(10) Don't cheat. Cheating will result in appropriate disciplinary action according to university policy.

PROBLEM 1 (45 points)

Consider the transport of a conservative tracer through a column of porous medium. The column has length $L = 50.0$ cm, porosity $n = 0.30$, radius $r = 2.5$ cm, cross-sectional area $A = \pi r^2 = 19.6$ cm^2, bulk density $\rho_b = 1.6$ g/cm^3, and longitudinal dispersivity $\alpha_L = 1.0$ cm. Water is pumped through the column at a volumetric flow rate $Q = 23.0$ cm^3/day. Initially, the column is devoid of any tracer: $C(x, t = 0) = 0$. However, at time $t = 0$, tracer is added to the column at the column inlet, at a concentration $C_0 = 10.0$ mg/L (i.e., a step concentration input). At time $t = 6.5$ days, here is what the concentration profile looks like, in graphical and tabular form:

x (cm)	C (mg/L)
0.	10.00
2.	10.00
4.	10.00
6.	9.99
8.	9.97
10.	9.93
12.	9.83
14.	9.65
16.	9.34
18.	8.87
20.	8.21
22.	7.34
24.	6.31
26.	5.18
28.	4.05
30.	2.99
32.	2.08
34.	1.36
36.	0.84
38.	0.48
40.	0.26
42.	0.13
44.	0.06
46.	0.03
48.	0.01
50.	0.00

Concentration Profile at t = 6.5 days
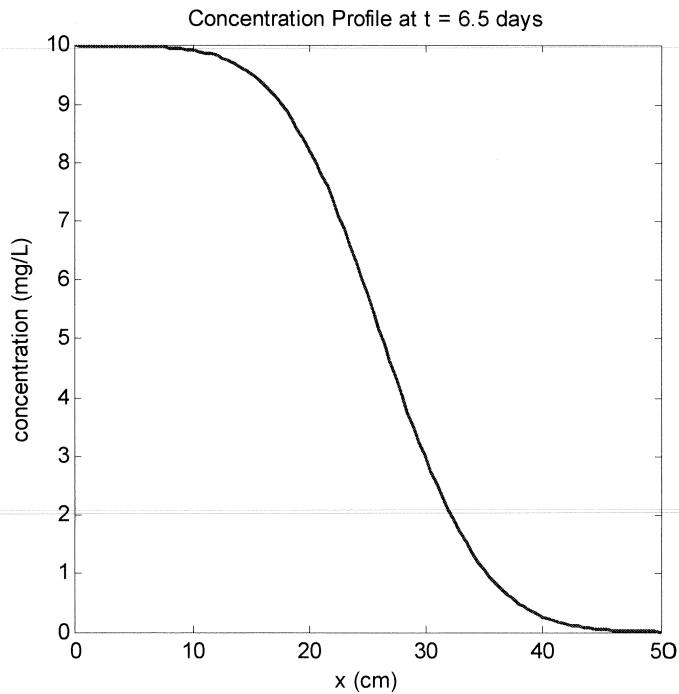
(a) (30 pts) Estimate/calculate/predict the tracer concentration at $x = 12.0$ cm at time $t = 7.5$ days. Report your answer to 2 decimal places (as in the table above). State your assumptions, show your work, and explain your reasoning, as necessary.

(b) (15 pts) Estimate/calculate/predict the tracer concentration at $x = 32.0$ cm at time $t = 7.5$ days. Report your answer to 2 decimal places. Hint: it will probably help you to do part (a) first.

PROBLEM 2 (20 points)

Two students are studying the transport of two hazardous chemicals (let's call them Compound 1 and Compound 2) through an aquifer comprised of unconsolidated sand and silt. The students acquire some sediment from the aquifer, and they use it to run some column experiments in the laboratory. The students fill two columns with the sediment. They attempt to build the two columns identically in terms of their transport properties (porosity, bulk density, length, etc.). The students use the two columns to run some transport experiments. In column 1, they measure the transport of Compound 1. In column 2, they measure the transport of Compound 2. Again, the students attempt to operate the two columns in an identical mode in terms of transport behavior -- same volumetric flow rate, same pore velocity, same mode of injecting the chemicals (step input), etc. In theory, the only difference between the two columns is that each one is for a different chemical. The students run their experiments, and measure the breakthrough curves (histories) of Compound 1 and Compound 2 in the two columns. Their results are shown here:

Concentration histories of Compound 1 and Compound 2

Solid line: Compound 1

Dashed line: Compound 2
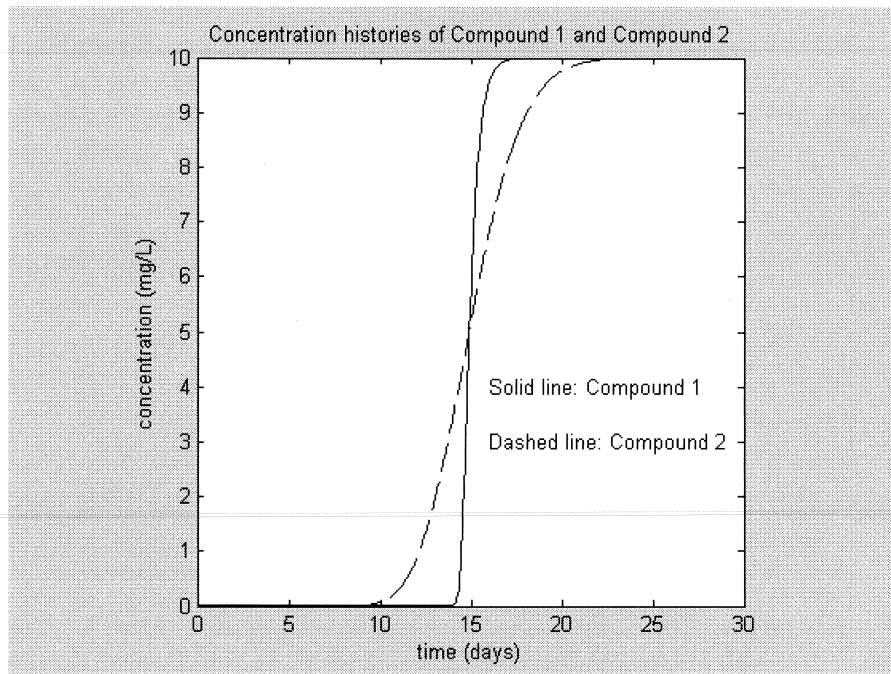
Upon seeing the results, Student 1 is disappointed. He says that these breakthrough curves indicate that they must not have built and/or operated their columns in an identical mode. Student 2 disagrees. He is convinced that they did build and operate their columns in an identical mode.

(a) (5 pts) Explain the reasoning of Student 1. Looking at the breakthrough curves, why would Student 1 think that the columns are not identical? What parameter(s) might be different between the two columns, in order to explain the experimental observations?

(b) (10 pts) Explain the reasoning of Student 2. If the two columns are, in fact, identical, then what other explanation(s) could there be for the observed differences? List all factors you can think of that could explain the experimental observations.

(c) (5 pts) Can you tell which of the two students is correct? If so, which one? If not, why not?

PROBLEM 3 (30 points)

All semester long, we have been studying the transport of contaminants through columns of porous media. It is not hard to take the principles and apply them to the transport of *heat* through porous media. Suppose we have a column filled with a porous medium, just as we have done all semester. The stationary solid phase might now be, say, ceramic spheres, instead of sand grains. The mobile fluid phase could be a liquid or a gas, but for simplicity, let's assume it is an incompressible liquid, like water. Then, the transport of heat through the column of porous medium can be described with this partial differential equation:

$$n\,\rho_w\,C_{p,w}\,\frac{\partial T_w(x,t)}{\partial t} + (1-n)\rho_g\,C_{p,g}\,\frac{\partial T_g(x,t)}{\partial t} \;=\; -q\,\rho_w\,C_{p,w}\,\frac{\partial T_w(x,t)}{\partial x} + n\,k\,\frac{\partial^2 T_w(x,t)}{\partial x^2}$$

where n is the porosity, ρ_w is the density of the water, ρ_g is the density of the solid grains, $C_{p,w}$ is the heat capacity of the water, $C_{p,g}$ is the heat capacity of the solid grains, q is the specific discharge of the fluid, k is the thermal conductivity of the water, T_w is the temperature of the water, and T_g is the temperature of the solid grains. Recall that $(1-n)\,\rho_g = \rho_b$, the bulk density of the solid phase in the column. (It is OK if you do not know what heat capacity and thermal conductivity are -- don't panic!)

This equation is based on a number of assumptions (for instance, the heat capacity and fluid density are both weak functions of temperature), but all the assumptions are reasonable, so the above equation is pretty good. The left-hand side of the equation represents accumulation of heat in the liquid and solid phases; the right-hand side represents the transport of heat by the processes of convection and conduction.

If we divide the whole equation through by the group of terms ($n\,\rho_w\,C_{p,w}$), then the equation becomes the following:

$$\frac{\partial T_w(x,t)}{\partial t} + \frac{(1-n)\rho_g\,C_{p,g}}{n\,\rho_w\,C_{p,w}}\frac{\partial T_g(x,t)}{\partial t} \;=\; -v\,\frac{\partial T_w(x,t)}{\partial x} + \alpha\,\frac{\partial^2 T_w(x,t)}{\partial x^2}$$

where v is the pore velocity of the water, and α is called the "thermal diffusivity" of the water.

Suppose that the column is 100 cm long with a porosity $n = 0.30$. Water is pumped through the column with a specific discharge $q = 6.0$ cm/day. Initially, the whole system is at a temperature of 10 °C:

$$T_w(x, t = 0) = 10\ °C$$
$$T_g(x, t = 0) = 10\ °C$$

Then, at time $t = 0$, there is a step increase in the temperature of the water that enters the column:

$$T_w(x = 0, t) = 40\ °C$$

or, in other words, hot water begins to displace the cold water starting at time $t = 0$. The density of water is $\rho_w = 1.0$ g/cm^3, the heat capacity of water is $C_{p,w} = 1.0$ cal/(g °C), and the thermal diffusivity of water is $\alpha = 120$ cm^2/day. Given this information, answer the following problems.

PROBLEM 3, continued

(a) (15 points) Suppose that the ceramic spheres do not absorb any heat as the hot water flows through the column. This is the same thing as saying that $C_{p,g} = 0$. In this case, draw a graph of the *temperature history* of the *water* at the location $x = 50$ cm. Also draw a graph of the *temperature profile* of the water at time $t = 2.5$ days. Label your axes, including units. Make your graphs quantitative if you can, but not *too* quantitative, because you have only about 15 minutes for this question.

(b) (15 points) Now assume that the ceramic spheres <u>do</u> absorb heat as the hot water displaces the cold water. In fact, the water and the spheres are always in rapid thermal equilibrium, such that $T_g(x,t) = T_w(x,t)$. The density of the ceramic spheres is $\rho_g = 2.0$ g/cm^3, and the heat capacity of the ceramic spheres is $C_{p,g} = 0.5$ cal/(g °C). Again draw the temperature history at $x = 50$ cm, and the temperature profile at $t = 2.5$ days.

PROBLEM 4 (10 points)

Explain, in your own words, the difference(s) between explicit and implicit numerical methods for solving the transport problem. What are the relative advantages and disadvantages of the two methods?

PROBLEM 5 (15 points)

Explain, in your own words, the difference(s) between the finite difference method and the finite element method for solving the transport problem. Be sure to indicate the basis or principle of each method as one of the differences you consider. What are the relative advantages and disadvantages of the two methods?

PROBLEM 1.

Conservative tracer in a column of porous media.

$L = 50.0$ cm, $\quad$ $n = 0.30$, $\quad$ $r = 2.5$ cm, $\quad$ $A = \pi r^2 = 19.6$ cm^2, $\quad$ $\rho_b = 1.6$ g/cm^3, $\quad$ $\alpha_L = 1.0$ cm

Water pumped through column at $Q = 23.0$ cm^3/day.

Initially $\quad$ $C(x, t=0) = 0$.

Then, step input at column entrance, $\quad$ $C(x=0, t) = C_0 = 10.0$ mg/L

Given concentration data at $\quad$ $t = 6.5$ days.

(a) Find concentration at $\quad$ $x = 12.0$ cm at $\quad$ $t = 7.5$ days.

Well, we could use either an <u>analytical</u> solution or a <u>numerical</u> solution for $C(x,t)$.

But we don't know all the boundary conditions, and we can't really compute error functions without a computer; so it will be difficult to use an analytical solution.

Therefore we can use a numerical solution. We're given data at $t = 6.5$ d, we want to know C at $t = 7.5$ days.

From our finite difference method, we know

$$\frac{C_j^{new} - C_j^{old}}{\Delta t} = D \frac{C_{j+1} - 2C_j + C_{j-1}}{\Delta x^2} - V \frac{C_{j+1} - C_{j-1}}{2\Delta x}$$

We can use an explicit method, an implicit method, or a Crank-Nicolson method to evaluate the spatial derivatives on the right-hand side. Implicit methods might be better, but they require the solution of a system of equations, so we'd probably better use an explicit method for this exam.

$$\frac{C_j^{new} - C_j^{old}}{\Delta t} = \frac{D}{\Delta x^2}\left[C_{j+1}^{old} - 2C_j^{old} + C_{j-1}^{old}\right] - \frac{V}{2\Delta x}\left[C_{j+1}^{old} - C_{j-1}^{old}\right]$$

or, re-arranging,

$$C_j^{new} = C_j^{old} + \frac{D\Delta t}{\Delta x^2}\left[C_{j+1}^{old} - 2C_j^{old} + C_{j-1}^{old}\right] - \frac{V\Delta t}{2\Delta x}\left[C_{j+1}^{old} - C_{j-1}^{old}\right]$$

So now we need D, Δt, Δx, and V.

PROBLEM 1, continued

(a) continued

Let's calculate v.

$$q = \frac{Q}{A} = \frac{23.0 \text{ cm}^3/d}{19.6 \text{ cm}^2}$$

$$v = \frac{Q}{nA} = \frac{q}{n} = \frac{(23.0 \text{ cm}^3/day)}{(0.3)(19.6 \text{ cm}^2)} = 3.91 \text{ cm}/day$$

$$D = \alpha_L v = (1.0 \text{ cm})(3.91 \text{ cm}/d) = 3.91 \text{ cm}^2/day$$

What about Δx? Well, we are given data in 2 cm intervals, so it makes sense to use $\Delta x = 2$ cm

That just leaves Δt.

We have data at $t = 6.5$ days, and we want C at $t = 7.5$ days, so it might make sense to use $\Delta t = 1.0$ days.

Then

$$\frac{D \Delta t}{\Delta x^2} = \frac{(3.91 \text{ cm}^2/d)(1.0 \text{ day})}{(2 \text{ cm})^2} = 0.978$$

$$\frac{v \Delta t}{2 \Delta x} = \frac{(3.91 \text{ cm}/d)(1.0 \text{ day})}{2(2 \text{ cm})} = 0.978$$

Thus

$$C_j^{new} = C_j^{old} + 0.978\left[C_{j+1}^{old} - 2C_j^{old} + C_{j-1}^{old}\right] - 0.978\left[C_{j+1}^{old} - C_{j-1}^{old}\right]$$

Notice that this simplifies because $\dfrac{D \Delta t}{\Delta x^2} = \dfrac{v \Delta t}{2 \Delta x}$

So we get $\quad C_j^{new} = C_j^{old} + (2)(0.978)\left[C_{j-1}^{old} - C_j^{old}\right]$

Given the data for $t = 6.5$ days, we get

$$C_j^{new} = 9.83 \frac{mg}{L} + (2)(0.978)\left[9.93 \frac{mg}{L} - 9.83 \frac{mg}{L}\right]$$

$$C_j^{new} = 10.03 \text{ mg}/L$$

Uh-oh !! This can't be right! We got $C > C_0$.
What happened?
We forgot that, with explicit methods, there can be stability and/or accuracy issues if Δt is too big.

PROBLEM 1, continued

(a) continued

So, let's check the stability criterion for this problem.
For the explicit Euler method,

$$\Delta t \leq \min\left[\frac{2D}{v^2}, \frac{\Delta x^2}{2D}\right]$$

because the method is only conditionally stable.
So from this, we get

$$\Delta t \leq 0.51 \text{ days}$$

Thus, to go from $t = 6.5$ days to $t = 7.5$ days, let's do two time steps, each of size $\Delta t = 0.50$ days.

$$\frac{D \Delta t}{\Delta x^2} = \frac{(3.91 \text{ cm}^2/d)(0.50\ d)}{(2 \text{ cm})^2} = 0.488$$

$$\frac{v \Delta t}{2 \Delta x} = \frac{(3.91 \text{ cm}/d)(0.50\ d)}{(2)(2 \text{ cm})} = 0.488$$

$$C_j^{new} = C_j^{old} + 0.488\left[C_{j+1}^{old} - 2C_j^{old} + C_{j-1}^{old}\right] - 0.488\left[C_{j+1}^{old} - C_{j-1}^{old}\right]$$

$$= C_j^{old} + 0.975\left[C_{j-1}^{old} - C_j^{old}\right]$$

So now find C at $t = 6.50\ d + 0.50\ d = 7.00$ days:

$$C(x=10, t=7) = 9.93 \text{ mg}/L + 0.975\left[9.97 \text{ mg}/L - 9.53 \text{ mg}/L\right] = 9.969 \text{ mg}/L$$

$$C(x=12, t=7) = 9.83 \text{ mg}/L + 0.975\left[9.93 \text{ mg}/L - 9.83 \text{ mg}/L\right] = 9.928 \text{ mg}/L$$

$$C(x=14, t=7) = 9.65 \text{ mg}/L + 0.975\left[9.83 \text{ mg}/L - 9.65 \text{ mg}/h\right] = 9.826 \text{ mg}/L$$

Now go from $t = 7.00$ days to $t = 7.50$ days

$$C(x=12, t=7.5) = 9.928 \text{ mg}/L + 0.975\left[9.969 \text{ mg}/L - 9.928 \text{ mg}/L\right]$$

$$= \boxed{9.97 \text{ mg}/L}$$

PROBLEM 1, continued

(b) Find the concentration at $x = 32$ cm at $t = 7.5$ days.

From part (a), we have the procedure all worked out already.

$$C_j^{new} = C_j^{old} + 0.975 \left[C_{j-1}^{old} - C_j^{old} \right]$$

So, going from $t = 6.5$ d to $t = 7.0$ d:

$$C(x = 30 \text{ cm}, t = 7) = 2.99 \frac{mg}{L} + 0.975 \left[4.05 \frac{mg}{L} - 2.99 \frac{mg}{L} \right] = 4.024 \frac{mg}{L}$$

$$C(x = 32 \text{ cm}, t = 7) = 2.08 \frac{mg}{L} + 0.975 \left[2.99 \frac{mg}{L} - 2.08 \frac{mg}{L} \right] = 2.967 \frac{mg}{L}$$

Then, go from $t = 7$ d to $t = 7.5$ d:

$$C(x = 32 \text{ cm}, t = 7.5 \text{ d}) = 2.967 \frac{mg}{L} + 0.975 \left[4.024 \frac{mg}{L} - 2.967 \frac{mg}{L} \right]$$

$$= \boxed{4.00 \text{ mg/L}}$$

NOTE: Just to check these estimates, I used our Crank-Nicolson computer code from class, using a small Δt and small Δx, and the boundary condition that $C(x = L, t) = 0$.

Then, the "right" answers are:

$$C(x = 12 \text{ cm}, t = 7.5 \text{ d}) = 9.94 \text{ mg/L}$$

$$C(x = 32 \text{ cm}, t = 7.5 \text{ d}) = 4.07 \text{ mg/L}$$

So the estimates from part (a) and (b) are not perfect, because we used a first-order-accurate method with a relatively large time step. Still, given the constraints of the exam, they are pretty good estimates.

PROBLEM 2

Two students are studying the transport of Compound 1 and Compound 2 through an aquifer. They get some aquifer sediment and build some columns in the lab. They try to make the two columns identical, except that Column 1 is for Compound 1, and column 2 is for Compound 2. When they measure the breakthrough, the two breakthrough curves look different. The two students disagree about why.

(a) Explain the reasoning of Student 1.

Student 1 thinks the columns must be different. The two compounds appear to break through at the same time, but one break-through curve looks more spread out than the other. Therefore, Student 1 would say that the columns had the same velocity, but different dispersion coefficients. Since $D = \alpha_L v$, this would mean that the two columns differed in their longitudinal dispersivity.

(b) Explain the reasoning of Student 2.

Student 2 maintains that the columns are identical. Therefore, any observed differences must be due to different chemistry, ie., different behavior of Compound 1 vs. Compound 2. There are two possibilities consistent with this theory:
   – perhaps Compound 1 undergoes non-linear sorption (favorable isotherm) while Compound 2 undergoes linear sorption. That would explain the sharp breakthrough of Compound 1.
   – perhaps Compound 1 undergoes equilibrium sorption, while Compound 2 undergoes non-equilibrium sorption, leading to more spread of the breakthrough curve for Compound 2.

In summary, the observed difference could be due to a difference in Peclet number, a difference in Damkohler number, or a difference in sorption isotherms.

PROBLEM 2, continued

(c) Which student is correct?

It is really impossible to tell (based on the given graph) which student is correct. If I had to guess, I'd say that it looks to me like non-linear (favorable) sorption of Compound 1 -- the shape of the curve just looks that way to me. But it could very easily be an effect of Pe or Da. I can't tell for sure who is correct.

PROBLEM 3

Let's study the transport of heat through porous media.

We can use the PDE

$$\frac{\partial T_w(x,t)}{\partial t} + \frac{(1-n)\rho_g C_{p,g}}{n \rho_w C_{p,w}} \frac{\partial T_g(x,t)}{\partial t} = -v \frac{\partial T_w(x,t)}{\partial x} + \alpha \frac{\partial^2 T_w(x,t)}{\partial x^2}$$

where all parameters are defined in the problem.

Suppose $L = 100$ cm, $n = 0.30$, $q = 6.0$ cm/day.

Initial condition $T_w(x, t=0) = 10°C$

$$T_g(x, t=0) = 10°C$$

Then, at $t=0$, a step increase in the influent water temperature

$$T_w(x=0, t) = 40°C$$

Given $\rho_w = 1.0$ g/cm³ $C_{p,w} = 1.0$ cal/(g °C) $\alpha = 120$ cm²/day.

(a) Suppose the solid phase absorbs no heat: $C_{p,g} = 0$
Draw temperature history and temperature profile.

If the solid phase absorbs no heat, such that $C_{p,g} = 0$ then
the PDE reduces to:

$$\frac{\partial T_w(x,t)}{\partial t} = -v \frac{\partial T_w(x,t)}{\partial x} + \alpha \frac{\partial^2 T(x,t)}{\partial x^2}$$

This looks just like the equation we've solved all semester!!
If the solid phase absorbs no heat, that is like a
contaminant transport problem where the sand grains absorb no
contaminant.

In other words, this problem is exactly analogous to the transport
of a conservative tracer!

We definitely know how to draw histories and profiles in that case.

Notice $v = \frac{q}{n} = \frac{6.0 \text{ cm/d}}{0.30} = 20 \frac{cm}{d}$

$\alpha = 120 \frac{cm^2}{d}$ $Pe = \frac{vL}{\alpha} = \frac{(20 \text{ cm/d})(100 \text{ cm})}{120 \text{ cm}^2/d} = 17$
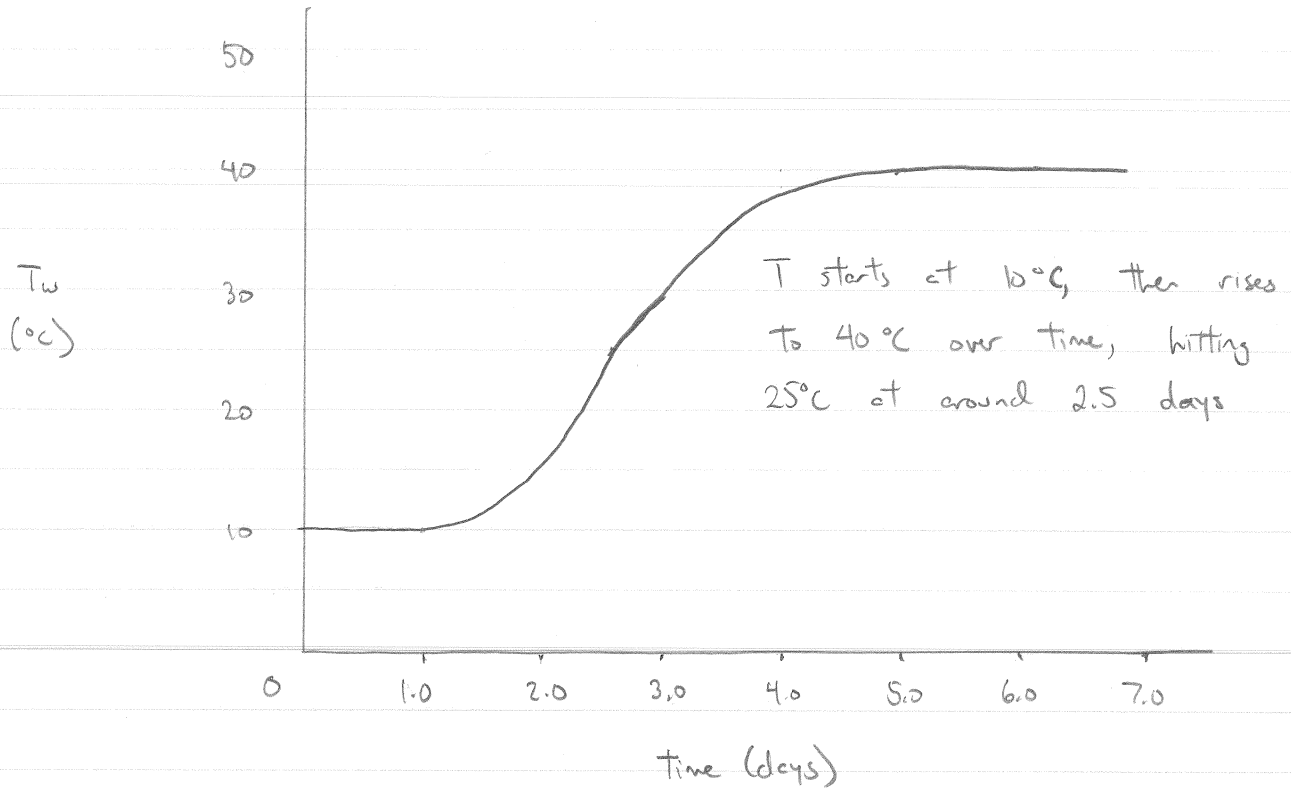
PROBLEM 3, continued

(a) continued.

Temperature history at x = 50 cm

Since v = 20 cm/d, it will arrive at about 2.5 days.

The Peclet number is relatively low (17), so there will be some measurable spread of the history.

I think it would look about like this:

T starts at 10°C, then rises to 40°C over time, hitting 25°C at around 2.5 days
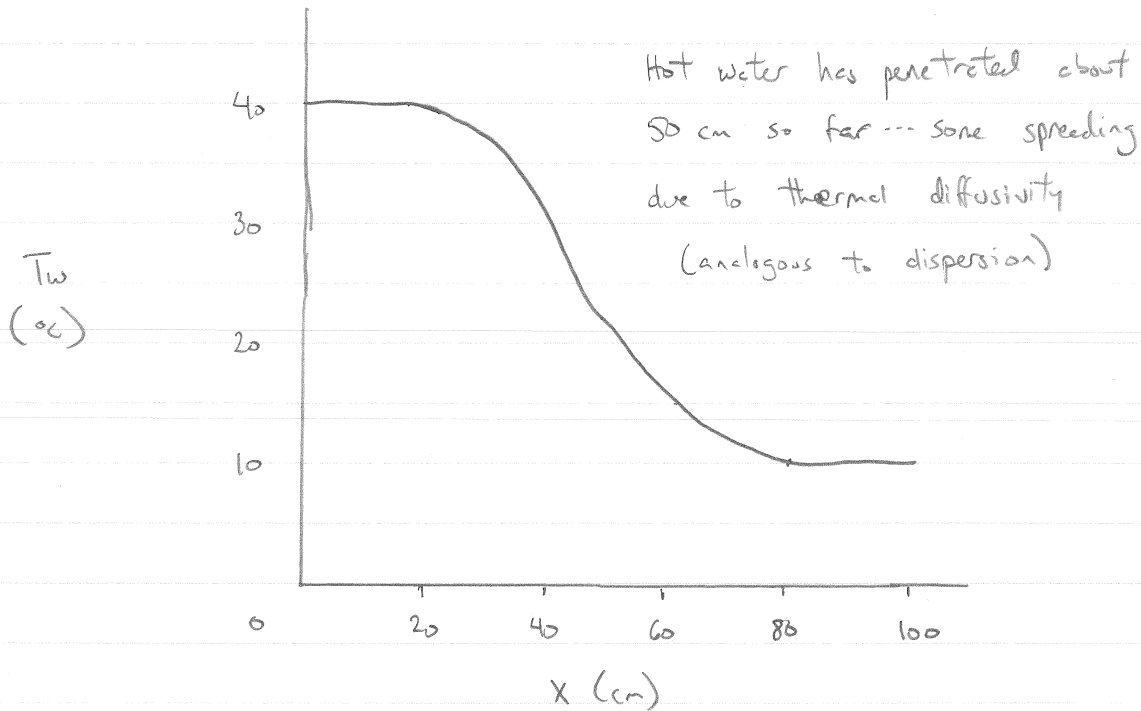
Temperature profile at t = 2.5 days

Since v = 20 cm/d, the hot water will have penetrated about 50 cm.

Again, dispersion will be appreciable.

See the graph on the next page.

PROBLEM 3, continued
(a) continued
Profile at t = 25 days:

Hot water has penetrated about
50 cm so far --- some spreading
due to thermal diffusivity
(analogous to dispersion)

(b) Now suppose the ceramic spheres do absorb heat. In fact, the
water and the spheres are in rapid thermal equilibrium, $T_g(x,t) = T_w(x,t)$.
Now draw the history and the profile.

The "rapid thermal equilibrium" is just like "local equilibrium!"
Saying $T_g(x,t) = T_w(x,t)$ is just like saying $S(x,t) = K_d \, C(x,t)$.
So we can calculate a retardation factor for the heat!
Since $T_g(x,t) = T_w(x,t)$, we also have

$$\frac{\partial T_g}{\partial t} = \frac{\partial T_w}{\partial t}$$

Therefore the PDE can be re-written as

$$\frac{\partial T_w(x,t)}{\partial t} \left\{ 1 + \frac{(1-n)\, \rho_g \, C_{p,g}}{n \, \rho_w \, C_{p,w}} \right\} = -v \frac{\partial T_w}{\partial x} + \alpha \frac{\partial^2 T_w}{\partial x^2}$$

PROBLEM 3, continued

(b) continued

So the retardation factor is

$$R = 1 + \frac{(1-n)\,\rho_s\,C_{p_{\text{s}}}}{n\,\rho_w\,C_{p_{\text{w}}}} = 1 + \frac{(0.67)(2.0\,{}^g/_{cm^3})(0.5\,\frac{cal}{g\,{}^{\circ}C})}{(0.33)(1.0\,{}^g/_{cm^3})(1.0\,\frac{cal}{g\,{}^{\circ}C})}$$
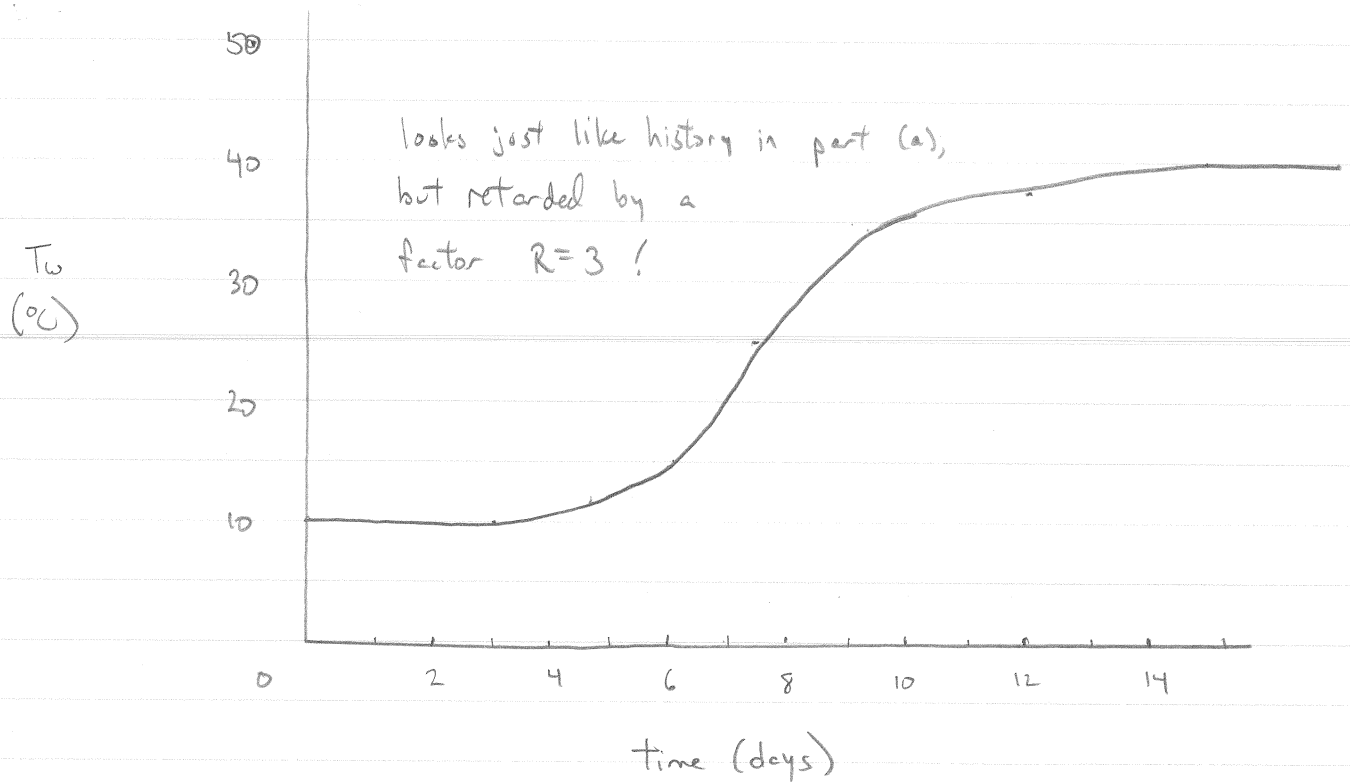
$$R = 3$$

Now we have

$$\frac{\partial T_w(x,t)}{\partial t} = \frac{\alpha}{R}\frac{\partial^2 T_w(x,t)}{\partial x^2} - \frac{v}{R}\frac{\partial T_w(x,t)}{\partial x} \qquad \text{where } R=3$$

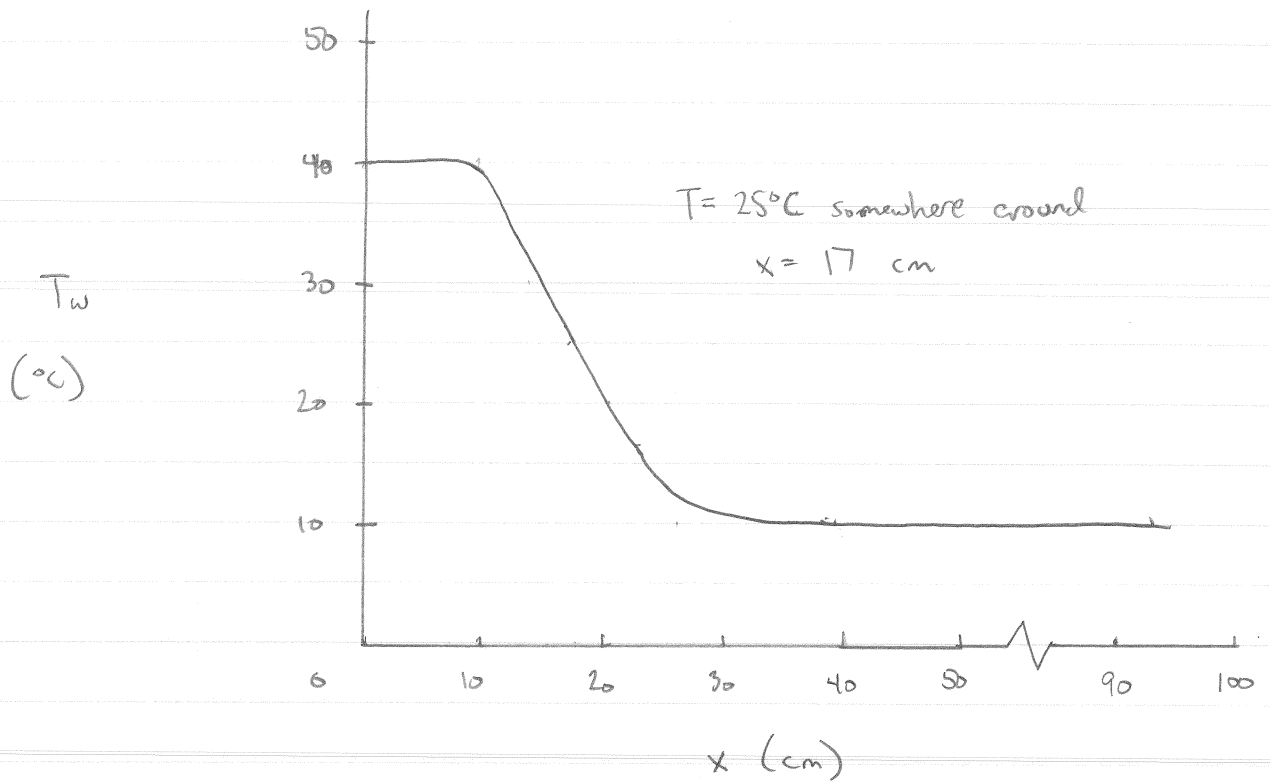This is just like contaminant transport with equilibrium sorption.
History at x = 50 cm

looks just like history in part (a),
but retarded by a
factor R=3!

PROBLEM 3, continued

(b) continued

   Profile at t = 2.5 days.

   Now the heat will have penetrated $\frac{vt}{R}$ = 17 cm instead of 50 cm

T = 25°C somewhere around
           x = 17 cm

PROBLEM 4

Explain the differences between explicit and implicit methods for solving the transport problem.

Both methods use knowledge of $C(x,t)$ to obtain an estimate of $C(x, t+\Delta t)$. They do this by solving a system of equations that usually looks something like this:

$$\frac{dC_j}{dt} = D\left[\frac{C_{j+1} - 2C_j + C_{j-1}}{\Delta x^2}\right] - v\left[\frac{C_{j+1} - C_{j-1}}{2\Delta x}\right]$$

Explicit methods evaluate the spatial derivatives on the right-hand-side at the beginning of the time steps i.e., at time t, when all values of C are known.

Implicit methods evaluate the spatial derivatives on the right-hand side at the end of the time step, i.e., at time $t+\Delta t$, when all values of C are unknown.

Therefore, explicit methods are easier to implement. Implicit methods require the solution of a system of algebraic equations for each time step. Implicit methods are harder to code and require more computations per time step.

However, explicit methods are only <u>conditionally</u> <u>stable</u>. Therefore a suitably small Δt (time step) is required. Implicit methods are <u>unconditionally stable</u> so that a larger Δt is generally allowable.

PROBLEM 5

Explain the differences between finite difference method and finite element method.

The finite difference method is based on approximating spatial derivatives with algebraic finite difference approximations:

$$\frac{\partial C}{\partial x} \approx \frac{C(x+\Delta x) - C(x-\Delta x)}{2\Delta x}$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C(x+\Delta x) - 2C(x) + C(x-\Delta x)}{\Delta x^2}$$

which allows the PDE to be converted to a system of ODE's:

$$\frac{\partial C(x,t)}{\partial t} = D\frac{C(x+\Delta x) - 2C(x) + C(x-\Delta x)}{\Delta x^2} - v\frac{C(x+\Delta x) - C(x-\Delta x)}{2\Delta x}$$

The finite element method is based on setting the integral of a weighted residual equal to zero. An approximate solution $\tilde{C}(x,t)$ is sought.

$$\frac{\partial \tilde{C}(x,t)}{\partial t} \approx D\frac{\partial^2 \tilde{C}(x,t)}{\partial x^2} - v\frac{\partial \tilde{C}(x,t)}{\partial x}$$

and the residual is defined:

$$\varepsilon(x,t) = \frac{\partial \tilde{c}}{\partial t} - D\frac{\partial^2 \tilde{c}}{\partial x^2} + v\frac{\partial \tilde{c}}{\partial x}$$

and the weighted residual is set equal to zero.

$$\int_0^L \varepsilon(x,t)\, f(x)\, dx = 0$$

Then, if we discretize the domain into <u>finite elements</u>, and define basis functions associated with those elements, we can seek an approximate solution of the form

$$\hat{C}(x,t) = \sum_{j=1}^{N+1} \phi_j(x)\, C_j(t)$$

where $\phi_j(x)$ are known basis functions and $C_j(t)$ are unknown nodal concentrations. This process again converts the PDE to a system of ODE's, something like:

$$\frac{1}{6}\frac{dC_{j-1}}{dt} + \frac{2}{3}\frac{dC_j}{dt} + \frac{1}{6}\frac{dC_{j+1}}{dt} = \frac{D}{\Delta x^2}\left[C_{j+1} - 2C_j + C_{j-1}\right] - \frac{v}{2\Delta x}\left[C_{j+1} - C_{j-1}\right]$$

Thus the two methods both result in systems of ODE's that look surprisingly similar, given how different the underlying principles appear.

The finite difference method is significantly easier to set up and turn into a computer code. However, we saw that the finite element method sometimes performs better, particularly in the case of high Peclet numbers (steep concentration fronts).