Chapter 3

Heat Conduction

3.1 September 24, 2003: Wrap up dimensional analysis, start heat conduction

Mechanics:

- Handout: heat conduction equation solutions.

- GE CEO tomorrow noon Bartos

- Tests 1, 2 (10/10, 11/19) first part in 2-143.

- Final Mon 12/15 1:30-4:30 "2-105"...

Muddy stuff from last time:

- How steady-state diffusion in oxide?

- How is $C_1 - C_0 = 2\frac{\rho}{M}$? $C_1 - C_0 \gg C_3 - C_1$ and $C_1 - C_0 \gg C_0$, so for this purpose, $C_1 = C_3$ =moles oxygen/unit volume in SiO_2 and $C_0 \simeq 0$. Molar density of SiO_2 is ρ/M, molar density of oxygen is twice that.

- Dimensional analysis was fast. Yes, learning the steps is easy, but "How to choose which variables to 'postulate desired behavior'?" Not easy, learn by example—we'll do this many more times this term...

- How to form dimensionless quantities? If counted $i = n - r$ correctly, and chose dimensionally-independent parameters to eliminate, then like simultaneous equations: units of J * (units of $\Delta C)^a$... etc. Table as an easier way of doing that. Will do an example today with π_k.

- (Multiple people) How is π_J a function of π_k? Stay tuned for the dramatic conclusion of dimensional analysis...

Dimensional Analysis Recap last time:

1. Postulate desired behavior as a function of the other variables, *e.g.* $J_O = f(C_1 - C_3, k, D, Y)$, or $f(J_O, C_1 - C_3, k, D, Y) = 0$. The number of parameters is n, in this case $n = 5$.

2. Find the number of base units in the system r. Here: cm, s, mol, so $r = 3$. (Rank of the dimensional matrix...)

3. Buckingham Pi theorem: number of dimensionless groups $= n - r$.

4. Choose r dimensionally-independent variables to eliminate, which will make the others dimensionless. Here we'll choose $C_1 - C_3$, D, and Y (NOT k, D and Y because they're not independent!)

5. Form the π groups from what's left, which are unitless versions of the parameters kept:

$$\pi_J = \frac{J_O Y}{(C_3 - C_1)D}, \pi_k = \frac{kY}{D}.$$

6. Rewrite Step 1 in dimensionless terms, and we're done: $\pi_J = f(\pi_k)$.

What's this? So simple? Can't be. Let's test:

$$J_O = \frac{C_3 - C_1}{\frac{1}{k} + \frac{Y}{D}}$$

Mult by $\frac{Y}{(C_3 - C_1)D}$ to give

$$\frac{J_O Y}{(C_3 - C_1)D} = \frac{1}{\frac{D}{kY} + 1} = \frac{1 + \frac{D}{kY} - \frac{D}{kY}}{\frac{D}{kY} + 1} = 1 - \frac{1}{1 + \frac{kY}{D}}$$

So,

$$\pi_J = 1 - \frac{1}{1 + \pi_k}$$

Limiting cases: large π_k means $\pi_J = 1 - 0 = 1$, so $J_O = \frac{D}{Y}(C_3 - C_1)$.

For small π_k, use $\frac{1}{1+x} \simeq 1 - x$ near $x = 0$, so $\pi_J = \pi_k$, $J_O = \frac{D}{Y}(C_3 - C_1)\frac{kY}{D} = k(C_3 - C_1)$. Excellent!

Purpose: simplify down to an easier expression, single graph. If couldn't solve equation, single graph could be obtained from one experiment, generalized to any other reaction-diffusion problem of the same nature. Physical modeling, e.g. wind tunnel: get the dimensionless numbers right, every detail of flow is the same, dimensionless drag force is identical!

Heat Conduction   Conservation of math (in one ear, out the other). But seriously, conservation of thermal energy, for us enthalpy. Usual equation:

$$\text{accumulation} = \text{in} - \text{out} + \text{generation}$$

$$V\frac{dH}{dt} = Aq_{\text{in}} - Aq_{\text{out}} + V\dot{q}$$

Note on the accumulation term: when temperature changes, enthalpy changes according to the heat capacity, build up units from dT/dt (Kelvin/sec) adding c_p and ρ to get to Joules/sec.

What's heat flux $\vec{q}$? Like diffusion goes down the conc gradient (actually, chem potential gradient), heat goes down the temperature gradient, proportionality constant k:

$$\vec{q} = -k\nabla T. \tag{3.1}$$

Using that in-out and that accumulation term, derive the 1-D heat equation, same as diffusion in section 2.5 (p. 20). Simplify constant k, 1-D, so:

$$\rho c_p \frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} + \dot{q}. \tag{3.2}$$

Define thermal diffusivity $\alpha = k/\rho c_p$, with no gen reduces to diffusion equation, and give 1-D solutions:

- 1-D steady-state: linear temperature.

- Cylindrical steady-state: $T = A\ln r + B$; with uniform generation: $T = A\ln r + B - Gr^2/2$

- 1-D semi-infinite uniform initial, constant T boundary:

$$\frac{T - T_s}{T_\infty - T_s} = \text{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right). \tag{3.3}$$

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- 1-D finite, uniform initial T, boundary constant T: Fourier series

$$\frac{T - T_s}{T_i - T_s} = \sum_{n=1}^{\infty} a_n \exp\left(-\frac{n^2\pi^2\alpha t}{L^2}\right) \sin\left(\frac{n\pi x}{L}\right) \qquad (3.4)$$

Even more on the handout, not responsible for any further than handout (and not asterisks either). Timescale to steady-state... any guesses?

Optional: Why does heat go down the temp gradient, and diffusion down the chem potential gradient? Thermo: increasing S or decreasing G. Spinodal decomposition: negative $\partial^2 G/\partial C^2$, uphill diffusion! Fourier series in reverse...

3.2 September 26, 2003: Heat conduction: boundary layers, multilayer wall

Opener: Christine Ortiz talk on how inquisitive this class is...
Mechanics:

- PS3 due today, PS4 due Monday 10/6.

- Last test 1 material next Wednesday, following math quiz in 2-143!

- Tests 1, 2 (10/10, 11/19) first part in 2-143.

- Final Mon 12/15 1:30-4:30 "2-105"...

- Zeiss materials microscopy truck at Chapel Turnaround 10/2 9-4.

Muddy from last time:

- Why is $\pi_J = \pi_k$ at small π_k? Okay. For $x \simeq 1$, $\frac{1}{x} \simeq 2 - x$. So, for $\pi_k \simeq 0$, $1 + \pi_k \simeq 1$, and

$$\frac{1}{1 + \pi_k} \simeq 2 - (1 + \pi_k) = 1 - \pi_k$$

$$\pi_J = 1 - \frac{1}{1 + \pi_k} \simeq 1 - (1 - \pi_k) = \pi_k$$

Boundary conditions

- Constant temperature.

- Constant flux $\vec{q} \cdot \hat{n}$ const, in 1-D $q_x = -k \frac{\partial T}{\partial x}$.

- Heat transfer coefficient: $q_x = h(T - T_{env})$. UNITS!

On the last, think about a boundary layer of thickness δ in a fluid, model h as k_f/δ. Then we can look at steady-state heat conduction through a plate, in particular the heat flux (T_1 BC on bottom, $h(T_2 - T_{env})$ BC on top):

$$q = \frac{k}{L}(T_1 - T_2) = h(T_2 - T_{env})$$

$$q = \frac{T_1 - T_{env}}{\frac{1}{h} + \frac{L}{k}}$$

Awesome! Now you know W^{3}R chapters 17 and 18—well, mostly.

Multilayer wall With lots of layers, just add up the resistances...

$$q = \frac{T_0 - T_n}{\frac{1}{h} + \frac{L_1}{k_1} + \frac{L_2}{k_2} + ... + \frac{L_n}{k_n} + \frac{1}{h_2}}$$

Same q_x everywhere implies that layers with higher k have lower $\partial T/\partial x$.

Cylindrical is slightly different, uses flux-area product, based on log solution:

$$Q = qA = \frac{2\pi L(T_1 - T_4)}{\frac{1}{k_1} \ln \frac{R_2}{R_1} + \frac{1}{k_2} \ln \frac{R_3}{R_2} + \frac{1}{hR_3}}$$

Temperature trick: use Biot number equivalent:

$$\frac{T_0 - T_2}{T_2 - T_n} = \frac{\text{resistances bet 2 and } n}{\text{resistances bet 0 and 2}}$$

3.3   September 29, 2003: Finally, the graphs!

Fun opener: typeset homework and course evaluation handwriting...
Mechanics:

- PS4 due Monday 10/6.

- Last test 1 material Wednesday, following math quiz in 2-143!

- Tests 1, 2 (10/10, 11/19) first part in 2-143.

- Final Mon 12/15 1:30-4:30 "2-105"...

- Zeiss materials microscopy truck at Chapel Turnaround 10/2 9-4.

Moddy from last time:

- How did we get:
$$q_x = \frac{T_1 - T_{fl}}{\frac{1}{h} + \frac{L}{k_s}}?$$
  Yes, skipped some steps because the math here is the same as the math for diffusion. See notes of 9/19 (section 2.7, page 24) for the derivation.

- Temperature for large Biot, small Biot...

- Albert: parallel composite wall...

- Blackboard technique...

Today's motivating example: powder metallurgy by spray/gas atomization. Small droplets, very rapid cooling, rapid solidification microstructures, solute trapping.

So, suppose initial condition $T = T_i$, outside fluid at T_{fl}. Boundary conditions: $r = R \Rightarrow q_r = h(T - T_{fl})$. Want to know temperature distribution through time, or temperature history. This requires a Bessel function series!! How to do understand?

- Dimensional analysis!

- Qualitative description of behavior.

- Graphs in text.

- Simpified low Biot number behavior: Newtonian cooling.

  Dimensional analysis:

1. Formulation: $T - T_{fl} = f(t, r, R, T_i - T_{fl}, h, k, \rho c_p)$. $n = 8$ parameters!

2. Base units: K, s, m, kg so $m = 4$.

3. Buckingham pi: four dimensionless parameters.

4. What to eliminate? Want to keep $T - T_{fl}$, t, r; choose h also. Eliminate R, $T_i - T_{fl}$, k, ρc_p.

5. π_T is easy, as is π_r. π_h: eliminated by k and R. π_t is funny, use k for seconds, ρc_p for Joules, R for remaining meters. Result is the Fourier number, the ratio of t/t_{SS}.

   Note: could have used h to eliminate seconds, but result wouldn't have been as cool: $\pi_t = ht/\rho c_p R$.

6. Dimensionless equation:
$$\frac{T - T_{fl}}{T_i - T_{fl}} = f\left(\frac{r}{R}, \frac{\alpha t}{R^2}, \frac{hL}{k}\right)$$

The solution to this requires a Bessel function series!! No simple solution we can fit to, so qualitative.

Now can graph π_T vs. π_r for various π_t, different graphs for different π_h. Large (> 100) reverts to the constant temperature boundary condition $T = T_{fl}$.

Had to end there, continuing after the Math Quiz on Wednesday...

3.4 October 1, 2003: Math Quiz, Graphs Wrapup, Newtonian Cooling

Mechanics:

- Zeiss Materials Microscopy Truck scheduled tomorrow: cancelled!

Muddy stuff:

- Mass transfer: diffusion/reaction-limited. Heat transfer: conduction/convection-limited. Mass transfer can also be convection-limited if we replace reaction constant k with mass transfer coefficient h_D.

Wrapup of The Graphs Now can graph π_T vs. π_r for various π_t, different graphs for different π_h. Large (> 100) reverts to the constant temperature boundary condition $T = T_{fl}$, small (< 0.1) we'll get to in a moment, intermediate Biot number graphs.

Newtonial cooling Small Biot number (< 0.1): temperture is roughly uniform. Let's say it *is* uniform. Then we just have $T(t)$, $\pi_T(\pi_t, \pi_h)$. Cool.

Balance over the entire object: accumulation = -out.

$$V\rho c_p \frac{dT}{dt} = -Aq_r = Ah(T - T_{fl})$$

Rearrange:

$$\frac{dT}{T - T_{fl}} = -\frac{Ah}{V\rho c_p}dt$$

Integrate, with initial condition T_i at $t = 0$:

$$\ln(T - T_{fl}) - \ln(T_i - T_{fl}) = -\frac{Aht}{V\rho c_p}$$

$$\frac{T - T_{fl}}{T_i - T_{fl}} = \exp\left(-\frac{Aht}{V\rho c_p}\right)$$

Plug in V/A:

- Sphere: $R/3$
- Cylinder: $R/2$
- Plate: "R" $= L/2$

Had to end there...

3.5 October 3, 2003: Moving on...

Mechanics:

- Test 1 next Friday 2-143; handout, answer any questions.

- Regular office hours; zephyrable (instance) most of next Tuesday.

- PS4 due next Monday 10/6, correction: #2a in BTU/hr not kW. Corrected version on Stellar.

- PS2#3c solution error: "at $t = 1$ second, $x = 9.6 \times 10^{-5}$cm, or just under one micron. At $t = 4$ seconds, $x = 1.92 \times 10^{-4}$cm, just under two microns." (was $\times 10^{-5}$...) Corrected version on Stellar.

- 3B Symposium Wednesday November 5.

Muddy from last time:

- What's this equation $V\rho c_p \partial T/\partial t = -Aq_r$? We've had that before, it looked like $V\partial H/\partial t = Aq_x|_x - Aq_x|_{x+\Delta x} + V\dot{q}$. I just skipped a step and went straight to accum=$V\rho c_p \partial T/\partial t$. Sorry about that.

- What's this bit about applying to different shapes? We left everything general, with volume and area, so whether a sphere, rod, plate, or crumpled up piece of paper, it just works.

The book takes a different approach to the graphs in Appendix F: π_T vs. π_t for various π_h, graphs at different π_r. Useful for temperature histories like PS4#3 (but skip past the early graphs...), and also for TTT diagrams, like our metal spray.

$$Y = \frac{T_\infty - T}{T_\infty - T_0} = f\left(X = \frac{\alpha t}{x_1^2}, n = \frac{x}{x_1}, m = \frac{k}{hx_1}\right)$$

Wrapup Newtonian cooling Last time we did accum $= - -$ out for the whole shape, got to:

$$\frac{T - T_{fl}}{T_i - T_{fl}} = \exp\left(-\frac{Aht}{V\rho c_p}\right)$$

First, examine terms, timescale, larger/smaller h, rho c_p, V/A. Plug in V/A:

- Sphere: $R/3$

- Cylinder: $R/2$

- Plate: "$R'' = L/2$

- Other shapes: varies...

Can instead define alternate Biot and Fourier numbers: Bi$' = \frac{hV}{kA}$, Fo$' = \frac{\alpha A^2}{V^2}t$, then:

$$\frac{T - T_{fl}}{T_i - T_{fl}} = \exp\left(-\frac{hV}{kA}\frac{kA^2}{\rho c_p V^2}t\right) = \exp\left(-\text{Bi}'\text{Fo}'\right)$$

So, all set for PS4, test1?

Thermal conductivity Diffusion is straightforward: atoms move, right? Well, not quite: gases in straight lines, liquid atoms move in chains, vacanices, interstitials, dislocations, etc. For heat, various mechanisms:

- Collisions

- Phonons

- Photons—radiation, which is spontaneous emission from hot body

- Electrons

On electrons, Wiedmann-Franz law:

$$k_{el} = L\sigma_{el}T, L = \frac{\pi}{3}(k_B/e)^2 = 2.45 \times 10^{-8}\frac{\text{Wohm}}{K^2}$$

where e=electron charge.

Metals: σ_{el} goes down with temperature. What about electrons is semiconductors?

Liquids: water .615 20-100°C, O_2 3.4×10^{-4}, H_2 1.77×10^{-3} (both 300K)

Influence of porosity and humidity/water absorption. Gases are very bad conductors, water not quite as bad but has very high specific heat! (PS4 #1d, water has four times c_p of aluminum which is highest there.)

Typical conductivity values: 0.1 to 300 $\frac{W}{m \cdot K}$. Porous→less, metals high, gases *really* small!

Note: at conference, diamond-aluminum composite for microelectronics, 45 vol% diamond but isotropic conductivity of 550 W/mK! Nearly twice copper, squeeze-castable into heat sink parts. Q: why no diamond-iron composite?

3.6 October 6, 2003: Finite Differences

Mechanics:

- Test 1 next Friday 2-143; handout, answer any questions.

- Regular office hours; zephyrable (instance) tomorrow 9-12, 1-5.

- Albert review session Thursday 7 PM in 8-302 (next door to recitation).

Muddy from last time:

- Why $\pi_T = \exp(-\pi_h' \pi_t')$ with no π_r? Because at low Biot number, T is uniform, not a function of r or π_r.

Finite differences   Very often no analytical solution to a system. (Or if there is one, it's impossibly complex.) So, use a computer, make some approximations.

- Discretize space: calculate temperature at a finite number of points on a grid (here 1-D). Choose x_i, calculate T_i. For simplicity, we'll choose evenly-spaced points, so $x_{i+1} - x_i = \Delta x$.

- Discretize time: calcluate temperature at a finite number of "timesteps" at times t_n, so with both, we have $T_{i,n}$. For simplicity, Δt uniform.

- Make some approximations about derivatives:

$$\left.\frac{\partial T}{\partial t}\right|_{x_i, t_{n+1/2}} \simeq \frac{T_{i,n+1} - T_{i,n}}{\Delta t}$$

$$\left.\frac{\partial T}{\partial x}\right|_{x_{i+1/2}, t_n} \simeq \frac{T_{i+1} - T_i}{\Delta x}$$

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{x_i, t_n} \simeq \frac{\left.\frac{\partial T}{\partial x}\right|_{x_{i+1/2}, t_n} - \left.\frac{\partial T}{\partial x}\right|_{x_{i-1/2}, t_n}}{\Delta x} \simeq \frac{T_{i-1,n} - 2T_{i,n} + T_{i+1,n}}{(\Delta x)^2}$$

So, let's look at the energy equation, and substitute approximations:

$$\frac{\partial T}{\partial x} = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c_p}$$

$$\frac{T_{i,n+1} - T_{i,n}}{\Delta t} = \alpha \frac{T_{i-1,n} - 2T_{i,n} + T_{i+1,n}}{(\Delta x)^2} + \frac{\dot{q}}{\rho c_p}$$

$$T_{i,n+1} = T_{i,n} + \Delta t \left[\frac{T_{i-1,n} - 2T_{i,n} + T_{i+1,n}}{(\Delta x)^2} + \frac{\dot{q}}{\rho c_p} \right] = T_{i,n} + \text{Fo}_M(T_{i-1,n} - 2T_{i,n} + T_{i+1,n} + \frac{\Delta t}{\rho c_p}\dot{q}$$

This is the "forward Euler" algorithm, a.k.a. "explicit" time stepping. Nice, efficient, easy to put in a spreadsheet. Problems: inaccurate because time and space derivatives not co-located, also unstable. Inaccuracy later.

Demonstrate instability for $\text{Fo}_M > \frac{1}{2}$:

$$T_{i,n+1} = T_{i,n}(1 - 2\text{Fo}_M) + 2\text{Fo}_M \frac{T_{i-1,n} + T_{i+1,n}}{2} + \frac{\Delta t}{\rho c_p}\dot{q}$$

So, it's like a weighted average between $T_{i,n}$ and the average of the two (show graphically). When $\text{Fo}_M > \frac{1}{2}$, the $T_{i,n}$ part is negative, so we shoot past it! So, the criterion is that it must be $\leq \frac{1}{2}$, larger timestep means less work, so use $\frac{1}{2}$.

Exercise: cut length step in half, for same total time, how many more timesteps? How much more computational work? Spreadsheet area...

To get rid of this instability, we have the "backward Euler" algorithm, a.k.a. "fully implicit" time stepping.

$$\frac{T_{i,n+1} - T_{i,n}}{\Delta t} = \alpha \frac{T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}}{(\Delta x)^2} + \frac{\dot{q}}{\rho c_p}$$

Cool! But, requires simultaneous equation solution for the next timestep. But it is unconditionally stable: infinite timestep means we solve the steady-state problem.

Solving the simultaneous equations:

$$-\mathrm{Fo}_M T_{i-1,n+1} + (1 + 2\mathrm{Fo}_M)T_{i,n+1} - \mathrm{Fo}_M T_{i+1,n+1} = T_{i,n} + \frac{\dot{q}\Delta t}{\rho c_p}$$

$$
\begin{array}{rcl}
T_{0,n+1} & = & T_{0,BC} \\
-\mathrm{Fo}_M T_{0,n+1} \quad + \quad (1 + 2\mathrm{Fo}_M)T_{1,n+1} \quad + \quad -\mathrm{Fo}_M T_{2,n+1} & = & T_{1,n} + \frac{\dot{q}_1\Delta t}{\rho c_p} \\
-\mathrm{Fo}_M T_{1,n+1} \quad + \quad (1 + 2\mathrm{Fo}_M)T_{2,n+1} \quad + \quad -\mathrm{Fo}_M T_{3,n+1} & = & T_{2,n} + \frac{\dot{q}_1\Delta t}{\rho c_p} \\
T_{4,n+1} & = & T_{3,BC}
\end{array}
$$

$$
\begin{pmatrix}
1 & & & \\
-\mathrm{Fo}_M & (1 + 2\mathrm{Fo}_M) & -\mathrm{Fo}_M & \\
& -\mathrm{Fo}_M & (1 + 2\mathrm{Fo}_M) & -\mathrm{Fo}_M \\
& & & 1
\end{pmatrix}
\begin{pmatrix}
T_0 \\
T_1 \\
T_2 \\
T_3
\end{pmatrix}
=
\begin{pmatrix}
T_{0,BC} \\
T_{1,n} + \frac{\dot{q}_1\Delta t}{\rho c_p} \\
T_{2,n} + \frac{\dot{q}_1\Delta t}{\rho c_p} \\
T_{3,BC}
\end{pmatrix}
$$

Now just use 18.06 matrix techniques: Gaussian elimination, LU decomposition, eigenvalues, etc.

3.7 October 8, 2003: More Finite Differences

Mechanics:

- Graded math quizzes back. Avg $96\frac{1}{4}$, std dev 4.85, 11 100s! Warm-up, next is the race.

- Test 1 next Friday 2-143; handout, answer any questions.

- Review session tomorrow 7 PM 8-302.

- I can have office hours Monday, but would much rather be available Wednesday 2:30-3:30.

- PS4 solution error: Newtonian cooling eq has just one t! Also in 10/1 and 10/3 lecture notes; corrections in Stellar and on Athena respectively.

Muddy from last time:

- Top and bottom rows in RHS last time were wrong, should have been $T_{0,BC}$ and $T_{3,BC}$. Sorry...

- "How... theoretically interesting.

  "You said you were going to start each lecture with a 'motivating factor'—a real example to tie things to so the lecture isn't just so many symbols and numbers—where was today's motivating factor?

  "I'm hoping to at least be able to see a problem being solved where all this is useful. Otherwise, this makes no sense, sorry."

  Okay, two examples today on the laptop.

Encourage to think of test as checkpoint, first evaluation (except Math quiz, but that doesn't count). And remember, you can make it up in the second sitting. Will not be straightforward, won't see PS problems, but will apply same techniques to new situations. You will have to think, but you can all do that, that's why you're here.

Finite differences Last time: Forward Euler/explicit, and Backward Euler/implicit timestepping. But both of these are integrating in time using the value at previous or next timestep. Like rectangles in numerical integration. Graphically show error as proportional to Δt. To increase accuracy, use trapezoids, right? Then error is proportional to $(\Delta t)^2$. That works like:

$$\frac{T_{i,n+1} - T_{i,n}}{\Delta t} = \alpha \frac{T_{i-1,n} - 2T_{i,n} + T_{i+1,n} + T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}}{2(\Delta x)^2} + \frac{\dot{q}_{i,n} + \dot{q}_{i,n+1}}{2\rho c_p}$$

This is "semi-implicit", or "Crank-Nicholson" time integration, also need to solve simultaneous equations.

Error goes as Δt^2 for Crank-Nicholson, Δt for explicit/implicit (forward/backward Euler), like trapezoid rule vs. simple rectangle Riemann integration.

2-D: two second derivatives in x and y, $T_{i,j,n}$ at x_i, y_j, t_n; explicit form:

$$\frac{T_{i,n+1} - T_{i,n}}{\Delta t} = \alpha \left(\frac{T_{i-1,j,n} - 2T_{i,j,n} + T_{i+1,j,n}}{(\Delta x)^2} + \frac{T_{i,j-1,n} - 2T_{i,j,n} + T_{i,j+1,n}}{(\Delta y)^2} \right)$$

With $\Delta x = \Delta y$, $\mathrm{Fo}_M = \alpha \Delta t / (\Delta x)^2$, we have:

$$T_{i,n+1} = (1 - 4\mathrm{Fo}_M)T_{i,j} + 4\mathrm{Fo}_M \frac{T_{i-1,j,n} + T_{i+1,j,n} + T_{i,j-1,n} + T_{i,j+1,n}}{4}$$

So the stability criterion is:

$$\mathrm{Fo}_m \leq \frac{1}{4} \Rightarrow \Delta t \leq \frac{\Delta x^2}{4\alpha}.$$

In 3-D:

$$\mathrm{Fo}_m \leq \frac{1}{6} \Rightarrow \Delta t \leq \frac{\Delta x^2}{6\alpha}.$$

Laptop spreadsheet demos: iron conduction ps5.gnumeric, freezing water lecture1008.gnumeric.

3.8   October 15, 2003: Moving Body

Mechanics:

- Test 1 a bit too long, which is average for me, but not good. Will aim for shorter next time.

- Test typo: m, n switch in equation sheet graph descr.

- Ambiguous wording in 4b: clarified on board, but take any self-consistent answer.

- Misleading wording in one test question! 2d: strike "—that is, what's a more realistic shape for this region".

- The graph: perhaps not big enough. Good news: after initial behavior, $\pi_t \propto \exp(-t)$ (works for Newt cooling always, $n = 1$ term of Fourier). So on log-linear graph, straight lines, can extrapolate.

- New version on Stellar (minus the graph), will be used in retake. Sorry!

- Office hours: Today 2:30-3:30.

- SOFCs and energy today 12:15 Marlar Lounge (37-252), Ashley Predith, MIT.

- Magnetic nanodots Monday 3-4 Chipman, Igor Roshchin, UCSD.

Moving body   Example: VAR of titanium alloys, nickel superalloys. Start, during operation. Nickel: 6-8 kA, 17→20"; Ti around 30 kA, 30→36".

Competition: thermal diffusion up vs. drive down. Suggest steady-state, sketch T vs. z.

Temperatures in ingot real complicated, flow, etc. But can analyze electrode now. Question: how much of the electrode is heated? What's the temperature profile?

Choose frame of reference of melt interface on the bottom of the electrode. Solid is moving with respect to frame of reference. Now conductive and convective heat fluxes: $\vec{q} + \rho c_p T \vec{u}$ (not really, but this is valid for the difference).

In and out have motion component! Important thing: in-out. in $= u_x \rho c_p T$, out too. Result when goes to zero:

$$\text{in} - \text{out} = -\frac{\partial}{\partial x}(q_x + \rho c_p T u_x)$$

This example: u_x, ρ, c_p are all constant, so we end up with:

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} - \rho c_p u_x \frac{\partial T}{\partial x} + \dot{q}$$

Rearrange slightly for constant $\rho c_p u_x$, substitute $q_x = -k \partial T / \partial x$:

$$\rho c_p \left(\frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} \right) = k \frac{\partial^2 T}{\partial x^2} + \dot{q}$$

Divide by ρc_p:

$$\frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c_p}$$

Discuss terms: why proportional to $\partial T / \partial x$, competing effects of positive $\partial^2 T / \partial x^2$ and negative $-\partial T / \partial x$. Graphical explanation.

What introductory math concept does this remind us of? The substantial derivative! Rewrite:

$$\frac{DT}{Dt} = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c_p}$$

Note that's the time derivative in the frame of reference of the moving solid. Cool!

Steady-state, no generation:

$$\alpha \frac{\partial^2 T}{\partial x^2} - u_x \frac{\partial T}{\partial x} = 0$$

Simple solution using the characteristic polynomial, $R = 0, u_x/\alpha$. Result:

$$T = A + B \exp\left(\frac{u_x x}{\alpha}\right)$$

Fit to boundary conditions: $x = 0 \Rightarrow T = T_M$, $x = \infty \Rightarrow T = T_i$ so use erf-style:

$$\frac{T - T_i}{T_M - T_i} = \exp\left(\frac{u_x x}{\alpha}\right)$$

Lengthscale=α/u_x. Graph, noting that u_x is negative. Titanium $\alpha = 0.1\frac{cm^2}{s}$, $u_x \sim 5\frac{cm}{min} = \frac{1}{12}\frac{cm}{s}$, so $\alpha/u_x = 1.2cm$, about 1/2 inch. So only the bottom few centimeters are heated at all, even at this low velocity!

Heat flux into the bottom:

$$q_x = -k\frac{\partial T}{\partial x} = -k(T_m - T_i)\frac{u_x}{\alpha}\exp\left(\frac{u_x x}{\alpha}\right) = -\rho c_p u_x(T_m - T_i)$$

Note $\rho c_p(T_m - T_i)$ is the enthalpy per unit volume to heat metal to its melting point. Mult by u_x for enthalpy per unit area to heat metal coming at a rate of u_x, which is a cool result.

Next time: heat flux required to melt...

3.9   October 17, 2003: Phase Change

Ask Andy re retake...
Mechanics:

- New version on Stellar (minus the graph), will be used in retake. Sorry!

- Test stats first time around: 62-86 within a std dev. But significant clustering, low 80s and low 60s.

Problem	Mean	Std. Dev.	Max
1.	5	0	5
2.	29.41	4.02	35
3.	22.34	7.21	34
4.	17.21	3.92	25
Total	73.97	12.34	94

- Yet another error: diffusion equation missing D!

- Magnetic nanodots Monday 3-4 Chipman, Igor Roshchin, UCSD. (Also mention interesting talk on Wednesday.)

- GLOAT ABOUT YANKEES!

Muddy from last time:

- Why $H = \rho c_p T$ in quotes? Well, $\Delta H = \rho c_p \Delta T$, for temperature change only. But $H = \rho c_p T$ is not true, show by graph.

- What is $H \cdot u_x$? That's the convective flux, the transfer of heat due to motion of a substance.

- Frames of reference: DT/Dt is the time rate of change for a particle moving with the solid (or later, fluid); $\partial T / \partial t$ is the time rate of change at a fixed point (in a certain frame).

- What's the significance of $q_x = -\rho c_p u_x (T_m - T_i)$? Well, $\rho c_p \Delta T$ is the heat per unit volume. How much heat to raise Ti from the initial temp to the melting point. Times u_x gives the heat/area/time, the flux required to raise titanium coming in at that speed. Think of u_x as meters/second, or as $\mathrm{m}^3/\mathrm{m}^2 \cdot \mathrm{s}$.

Phase change   Another important concept: heat generated/lost at interface due to phase change. If extend the graph beyond $x = 0$ into liquid, more flux from liquid into interface than from interface into solid. How much more?

$$q_{x,l} - q_{x,s} = -\rho \Delta H_M u_x$$

Example: candle, MIT undergrad; "Build a man a fire..."

    Model of casting limited by conduction through metal, per Albert's recitation; graphical representation on board. Analogy to diffusion phase change (silicon oxidation): H is like C, T is like chemical potential μ. Fast growth means proportional to undercooling (ask Albert), like reaction-limitation in oxidation.

Evaporation/condensation   Also for evaporation, heat flux from gas, plasma, radiation incl. laser (below), electron beam, etc. Condensation releases heat at a similar rate.

    Evaporation into gas: boundary layer, $J = h_D (C_s - C_{bulk})$.

    Evaporation rate into a vacuum: Langmuir equation

$$J = \frac{p_v}{\sqrt{2\pi MRT}}$$

Here the units should work, go through.

    Equilibrium pure vapor pressure: Clausius-Clapeyron equation, one form:

$$\log_{10} p_v = -\frac{A}{T} + B + C \log_{10} T (+DT)$$

Units: torr, conversion factor. If not pure, then mult by activity. Either way, multiply material flux J by ΔH_{vap} for heat flux influence.

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3.10 October 20, 2003: Radiation

Mechanics:

- Test stats first time around: 62-86 within a std dev. But significant clustering, low 80s and low 60s.

Problem	Mean before	Std. Dev.	Max
1.	5	0	5
2.	29.41	4.02	35
3.	22.34	7.21	34
4.	17.21	3.92	25
Total	73.97	12.34	94

- Magnetic nanodots today 3-4 Chipman, Igor Roshchin, UCSD.

Evaporation cont'd: When to use dense gas, line-of-sight vacuum approxes? Mean free path λ:

$$\lambda = \frac{1}{\sqrt{2}\pi\sigma^2 n}$$

σ is collision diameter, n is number of molecules per unit volume, $P/k_B T$ (sketch molecules). Important thing is the Knudsen number, λ/L, given by:

$$\text{Kn} = \frac{\lambda}{L} = \frac{kT}{\sqrt{2}\pi\sigma^2 PL}$$

so in $P - T$ space, lines deliniate "line-of-sight" régime (Kn>1), "continuum" régime (Kn<0.01).

Radiation! Def: spontaneous emission of photons from a hot body. Emission, absorption, reflection, transmission. Cosine distribution: hand-waving skin depth explanation.

Happens throughout a body, but surface emission follows a cosine distribution: handwaving explanation of skin depth as a function of angle.

Concept: black body, absorbs all incident radiation, theoretical construct with some practical application. Also emits maximum possible radiation. Handwaving explanation: zero reflection at the interface.

Defs: e is power emitted per unit area, e_b is power emitted by black body per unit area, e_λ is power per unit wavelength per unit area, $e_{b,\lambda}$ is power by black body per unit wavelength per unit area.

Emission spectrum of black body:

$$e_{b,\lambda} = \frac{2\pi hc^2\lambda^{-5}}{e^{\frac{ch}{k_B\lambda T}} - 1}$$

h is Planck's constant, c is light speed, k_B Boltzmann's constant. Graph for different T.

How to get e_b? Integrate over all wavelengths. Fortunately, it's quite simple:

$$e_b = \int_0^\infty e_{b,\lambda} d\lambda = \sigma T^4$$

The physicists must have jumped for joy when they saw that one. For our purposes, it puts radiation within reach of engineers. Okay, all done, never have to see that first equation again.

Even better:

$$\sigma = \frac{2\pi^5 k_B^4}{15c^2 h^3} = 5.67 \times 10^{-8} \frac{\text{W}}{\text{m}^2 \cdot \text{K}^4}$$

Note: fourth-power dependence on temperature means this is **MUCH** more important at high temperature than low temperature.

New defs: emissivity $\epsilon_\lambda = e_\lambda/e_{b,\lambda}$, the fraction of black body radiation which is emitted; absorptivity $\alpha_\lambda = a_\lambda/a_{b,\lambda}$. Cool result: $\epsilon_\lambda = \alpha_\lambda$, always! Material property. Graph resulting emission spectrum.

Grey body approximation: $\epsilon = \alpha = \epsilon_\lambda = \alpha_\lambda = $ constant. Makes life a lot simpler for us engineers. Superpose grey spectra on previous graph.

Resulting emission: $e = \epsilon\sigma T^4$. Pretty cool. Likewise average absorptivity α.

Real materials: $\epsilon = f(T)$, $\alpha = f(\text{incident spectrum})$. Example: global warming, CO_2 absorbs in the infrared, admits sun in visible.

3.11   October 22, 2003: More Radiation

Mechanics:

- CONGRATS TO ALBERT!

- Test stats first time around: 62-86 within a std dev. But significant clustering, low 80s and low 60s.

Problem	Mean before	Std. Dev.	Max	Mean after	Std. dev	Max
1.	5	0	5	5	0	5
2.	29.41	4.02	35	34.66	0.86	35
3.	22.34	7.21	34	33.83	1.49	35
4.	17.21	3.92	25	24.59	1.02	25
Total	73.97	12.34	94	98.07	2.36	100

   "A" I consider around 80/89, because of statistics. Did well, 20%; not so well, only 20%.

- Subra on bionano cell mechanics next Monday 4PM 10-250. Recruiting...

Muddy from last time:

- Why is ϵ a function of T? Semiconductor example: silicon has band gap, absorbs some near infrared and in visible and higher energy (lower wavelength), very little in far infrared. So at low T, low ϵ; at higher T (up to melting point), higher ϵ. Note: can't be heated by IR heat lamp. Also note: liquid silicon has zero band gap!

   Peak wavelength:
$$\lambda_{max}T = 2.9 \times 10^{-3} \text{m} \cdot \text{K}$$

1000K, 2.9μm=2900 nm; sun at 5800K is at 500 nm (yellow)—need to be pretty hot to peak in the visible spectrum.

   Little table:

	Wavelength	Total/average
BB Emission	$e_{b,\lambda}$	$e_b = \int_0^\infty e_{b,\lambda}d\lambda$
Actual emission	e_λ	$e(=q) = \int_0^\infty e_\lambda d\lambda$
Emissivity	$\epsilon_\lambda = e_\lambda/e_{b,\lambda}$	$\epsilon(T) = e/e_b$
Absorptivity	$\alpha_\lambda \equiv \epsilon_\lambda$	$\alpha(incident)$

   Fortunately e_b is quite simple:

$$e_b = \int_0^\infty e_{b,\lambda}d\lambda = \sigma T^4, \sigma = 5.67 \times 10^{-8} \frac{W}{m^2 \cdot K^4}$$

Grey approximation means we stick an average ϵ in there. Note: fourth-power dependence on temperature means this is **MUCH** more important at high temperature than low temperature.

   Averaged properties: $\epsilon = e/e_b$, $\alpha = a/incident$. Note ϵ will vary with temperature, α depends on wavelength of incident light.

Radiation viewfactors   So, the pointof radiative exchange: how much radiation emitted by surface 1 reaches surface 2? Double integral:

$$Q_{12} = \int_{S1}\int_{S2} \frac{e_1 \cos\theta_1 \cos\theta_2}{r^2}dA_2 dA_1$$

A really ugly thing!

   Okay, but suppose A is at a uniform temperature, B also? Then can pull out e_A, α_B; define F_{12}:

$$Q_{12} = e_1 \int_{S1}\int_{S2} \frac{\cos\theta_1 \cos\theta_2}{r^2}dA_A dA_B$$

$$Q_{12} = e_1 A_1 F_{12}$$

F_{12} is only a function of the shape, not the size; is dimensionless.

Viewfactor Algebra: two principles

$$A_1 F_{12} = A_2 F_{21}$$

Prove from equal temperature.

$$\sum_{i=1} n F_{ji} = 1$$

if they form an enclosure. Simple thing. With these two, can do complex stuff. Simple geom graphs on pp. 396–398. Note: $F_{11} \neq 0$ if concave.

For coaxial disks of same radius, graph F_{12} vs. d/r, values below.

Example: disk and cylinder section height d/4 to d/2 above, viewfactor for disks d/4 is 0.6, for d/2 is 0.375. Derive $F_{21} = 0.225$ by enclosure arguments; $F_{12} = \frac{A_2}{A_1} F_{21} = F_{21}$ by this argument.

Total exchange viewfactor: NOT COVERED THIS YEAR Reflection can be specular, diffuse. Here discuss diffuse. Suppose two grey bodies forming an enclosure, diffuse reflection at same cosine distribution.

$$Q_{12,net} = e_{b1}\epsilon_1 A_1 F_{12}(1-\epsilon_2)A_2 F_{21}(1-\epsilon_1)A_1 F_{12}\text{etc.} - e_{b2}\epsilon_2 A_2\text{etc.}$$

Simplifies to:

$$Q_{12,net} = \frac{e_{b1} - e_{b2}}{\frac{1-\epsilon_1}{A_1\epsilon_1} + \frac{1}{A_1 F_{12}} + \frac{1-\epsilon_2}{A_2\epsilon_2}}$$

Funny thing: like a sum of resistances. Funnier stil: multiple surfaces forming an enclosure $\Rightarrow$ resistance diagram!

New concept: zero-flux surface, well-insulated, reflected+emitted$\simeq$incident. In that case, no "current" through that resistor, can get the total from surface 1 to 2 bypassing surface R. Pretty cool!

Total Exchange Viewfactor: $\bar{F}_{12}$, in this case

$$A_1 \bar{F}_{12} = A_1 F_{12} + \frac{1}{\frac{1}{A_1 F_{1R}} + \frac{1}{A_2 F_{2R}}}$$

Substitute that in instead of $A_1 F_{12}$ in $Q_{12,net}$ equation above.

Done with radiation, with heat transfer, on to fluids!