3.185 Lectures

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Abstract

This represents the sum total of lecture material presented in 3.185, *Transport Phenomena in Materials Engineering*, in the Fall of 2003. It is not meant to be a "reader" for the course, but more of an "electronic notebook" of my own, a set of bullet points if you will, to guide the content of each lecture. As such, it reads very poorly, but does contain all of the equations and derivations presented in the course.

Contents

Chapter 1

Introduction

1.1 September 3, 2003

Handouts: syllabus, ABET, Diffusion, PS1 due Monday 9/8.

Circulate signup sheet: name, username, year, course

- Introductions: me, Albert.
- What is covered: review stuff on general overview. Lots of complexity: from single ODE to five fully-coupled nonlinear second-order PDEs in five field variables.
- Intro to the general transport methodology: conservation and constitutive equations

  $$\text{accumulation} = \text{in} - \text{out} + \text{generation} \tag{1.1}$$

  Discuss the "terms", with a flying eraser.

  Microscopic and macroscopic.
- Necessary for all classes of materials, ask how many are interested in each:
  - Polymers: synthesis, injection molding, membranes (Bo)
  - Bio: drug delivery, anisotropic diffusion, blood flow (cool)
  - Ceramics: powder synthesis, separation, drying, sintering
  - Electronic: crystal growth, CVD, diffusion
  - Metals: smelting, refining, casting, heat treatment
- Why 3.185 is important: processing-(structure)-properties-performance. We do low-cost, high-quality processing, low environment overhead, which is one of the two important aspects of this triad/tetrahedron.

  Sponsors of our work care about two things: low-cost high-quality processes and high performance. They don't care about structure. Andy Groves, chairman of Intel, could care less about the electronic structure of titanium silicide-titanium aluminide diffusion barriers in aluminum interconnects, he wants cheap high-quality processes that result in high performance. Closer to home, parents' eyes glaze over at talk of "Kinetics of eta phase precipitation in nickel superalloys," but not at "Avoiding catastrophic failure of jet engine turbine blades in service." Structure provides an important way to model the relationship between processing and properties, without which a black box, not a science.

Mechanics

- Discuss grading: HW points and collab, double-session tests, mixed final.
- Get test conflict dates, aim for Weds. 10/15–17, 11/19–21.
- Make sure everyone has a recitation.
- Schedule office hours.
- Discuss travel: three trips, none of which should impact 3.185. If one more, tradition of having previous TA give a lecture.

Required math

- Vector arithmetic (dot product, cross product, outer product)
- Vector calculus (gradient, divergence, curl)
- Solving homogeneous linear ordinary differential equations, e.g.

$$y'' = k, \quad \text{or} \quad y'' - ky = 0 \tag{1.2}$$

- What partial differential equations look like, e.g.

$$\nabla^2 C = 0 \tag{1.3}$$

- The error function and derivatives:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi \tag{1.4}$$

$$\frac{d}{dx}\operatorname{erf}(x) = \frac{d}{dx}\frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi = \frac{2}{\sqrt{\pi}} e^{-x^2} \tag{1.5}$$

- The substantial derivative: the time derivative in a moving frame.

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla \tag{1.6}$$

  Kind of like moving vector $x(t), y(t), z(t)$:

$$\left.\frac{dC}{dx}\right|_{(x,y,z)} = \frac{\partial C}{\partial t} + \frac{\partial C}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial C}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial C}{\partial z}\frac{\partial z}{\partial t}. \tag{1.7}$$

Previous feedback

- Prof. Powell is cool, lectures are great, double tests are neat!
- This course spent way too much time on diffusion. Okay, will cut a bit shorter this time. But non-3.01s will be lost, need to see TA or me.
- Too much busy algebra on problem sets. Okay, will cut quite a bit, some computer.
- Problem sets should be due on Friday instead of Monday, for last-minute recitation help. Poll class, incl. PS1 Mon or Weds?
- Textbook is awful. It covers things in the wrong order, and is hard to read. Changing to new textbook, better readings, but still wrong order. Also see Incropera and DeWitt, in Reading Room; old text there too.

- TLL: “muddiest part”, index cards for each lecture from Friday, started last year, need more.
- Too much online. But taking it off would only hurt those without Bibles. Sorry, won’t do.
- Prof. Powell lets “dumb” questions slow things down. No dumb questions. Very often correct mistakes or omissions, ten others have the same question. If anything, MIT juniors and seniors need to be much more vocal! (Last mid-term evaluation, dreadful lecture...)

Chapter 2

Diffusion

2.1 September 5, 2003: 1-D Cartesian and Cylindrical Steady-State

TODO:

- Check reading room to make sure texts are there.
- Bring: cards, class list.
- Check text to make sure chap 25 units are consistent with mine.

Opener: Colleen's facility with names... my advisee!

Mechanics:

- Diffusion handout typo: should be erfc(y) = 1–erf(y).
- Choose new recitation times!
- Finalize test dates.
- Invite example processes.
- Index cards for muddiest part.
- Try names.

Diffusion Stuff they've learned before, new twist. Steady state 1-D cartesian, cylindrical coordinates.

Steady-state: accumulation=0. In today's case, species isn't generated or consumed inside the glass, so in–out=0. (Monday: generation by homogeneous chemical reaction.)

1-D: concentration varies only in one direction.

My style: start with a motivating example, introduce the physics along the way. When we're done, we have the physics, and an example of how to use it.

Yesterday: 3.185 is about low-cost high-quality processes. Here a process, not for material but for helium, maximize productivity a.k.a. throughput subject to process constraints.

Example: helium diffusion through pyrex glass, enormously higher D than any other gas (25x hydrogen!). Some helium in natural gas, can flow through pyrex tubes to separate, 2mm OD 1mm ID. Generally diffusion-limited. Want to calculate the production rate, more important understand how works, because from understanding flows design recommendations. ASSUME diffusion-limited, so this is the slow-step, not adsorption/desorption etc.

Simple solution: unroll to a plate, with C_{in} on one side (equilibrium with partial pressure in natural gas) and C_{out} on the other (pumped away into tanks), be sure to use thickness δ. We know how to do this:

Constitutive law: Fick's first, gradient points up, diffusion goes down, proportionality constant D:

$$\vec{J} = -D\nabla C, J_x = -D\frac{\partial C}{\partial x} \tag{2.1}$$

Units of each term.
1-D: no difference in y- or z-direction, so those partials are zero. When varies in only one direction and not time, not partial but total dC/dx.
Conservation with no accumulation or generation: $dJ_x/dx = 0$, substitute to get

$$\frac{d}{dx}\left(D\frac{dC}{dx}\right) = 0, \tag{2.2}$$

ASSUME constant D this is

$$\frac{d^2C}{dx^2} = 0. \tag{2.3}$$

General solution in 1-D:

$$C = Ax + B. \tag{2.4}$$

Boundary conditions (limited by diffusion):

$$x = 0 \Rightarrow C = C_{in}, x = \delta \Rightarrow C = C_{out}. \tag{2.5}$$

Result: flux

$$J = -DdC/dx = -D\frac{\Delta C}{\delta}. \tag{2.6}$$

At 500°C, $D_{\text{He}-\text{pyrex}} = 2 \times 10^{-8}\ \frac{\text{cm}^2}{\text{s}}$, for some steady gas/helium mixture $C_{in} = 10^{-5}\frac{\text{g}}{\text{cm}^3}$, say $C_{out} \simeq 0$. For $\delta = 0.5\text{mm} = 0.05\text{cm}$, this gives

$$J = 2 \times 10^{-8}\ \frac{\text{cm}^2}{\text{s}} \cdot \frac{10^{-5}\frac{\text{g}}{\text{cm}^3}}{0.05\text{cm}} = 4 \times 10^{-12}\frac{\text{g}}{\text{cm}^2 \cdot \text{s}}. \tag{2.7}$$

Tube array with total length 10m=1000cm (e.g. 100 tubes each 10 cm long), $R_2 = \text{OD}/2 = 0.1\text{cm}$, so throughput is

$$JA = 2\pi R_2 L J = 8 \times 10^{-10}\pi = 2.5 \times 10^{-9}\frac{\text{g}}{\text{s}} \tag{2.8}$$

Or do we use R_1? That would give 1.2×10^9. How far off is the flux? A dilemma.
Timescale: $\delta^2 \simeq Dt \Rightarrow$ steady state. Here $t \simeq \delta^2/D = 125000$ seconds, about a day and a half.

Design: what to do to improve throughput?

- Smaller δ: possible breakage
- Higher D: change glass, raise temperature
- Higher ΔC: raise/lower temperature, change glass

Okay, that was the braindead 1-D solution. What about the real cylinder?

Cylindrical coordinates So, C_{out} at outside, C_{in} at inside, what to do between? Use R_1 and R_2 for inner, outer radii. Fick's first, assume 1-D, so C is function of r only.

$$J_r = -D\frac{dC}{dr} \tag{2.9}$$

Conservation: in at $r + \Delta r$, out at r, no gen or accum, area $2\pi rL$:

$$0 = [2\pi rLJ_r]_r - [2\pi rLJ_r]_{r+\Delta r}, \tag{2.10}$$

divide by $2\pi L$, $\Delta r \to 0$:

$$0 = -\frac{d}{dr}[rJ_r] \tag{2.11}$$

Plug in flux:

$$0 = \frac{d}{dr}\left(rD\frac{dC}{dr}\right). \tag{2.12}$$

Now solve:

$$\begin{aligned}
A' &= rD\frac{dC}{dr} && (2.13)\\
\frac{A'}{Dr} &= \frac{dC}{dr} && (2.14)\\
C &= A\ln r + B && (2.15)
\end{aligned}$$

where $A = A'/D$. From BCs:

$$\frac{C - C_{in}}{C_{out} - C_{in}} = \frac{\ln(r/R_1)}{\ln(R_2/R_1)} \tag{2.16}$$

Check at R_1 and R_2, units.
Flux$= -DdC/dr$:

$$J_r = -D\frac{dC}{dr} = -D\frac{d}{dr}\left[C_in + (C_{out} - C_{in})\frac{\ln(r/R_1)}{\ln(R_2/R_1)}\right] = D\frac{C_{in} - C_{out}}{\ln(R_2/R_1)}\frac{1}{r}. \tag{2.17}$$

Important result: not flux, but flux times area.

$$AJ_r = -2\pi rLD\frac{dC}{dr} = 2\pi rLD\frac{C_{in} - C_{out}}{\ln(R_2/R_1)}\frac{1}{r}. \tag{2.18}$$

Note rs cancel, so AJ_r is constant for all r. Make sure units work. Cool.
Numbers, result: 1.8×10^{-9}. Between the 1-D estimates. Overestimated flux, at R_2 is really 1.44×10^{-12}, twice that at R_1, so R_1 value is closer.
More important: cartesian gave *wrong design criterion*! Not minimize δ, but minimize R_2/R_1! Double production by going from 2 to $\sqrt{2}$ because $\ln(\sqrt{2}) = \frac{1}{2}\ln(2)$, e.g. 3 mm OD with no change in thickness!
Other design issues: helium on inside or outside? Inside means glass is in tension, outside compression. But if gas is dirty, inside is easier to clean.
Note: on problem set 2, will derive this for a sphere for a drug delivery device. Pretty cool.

2.2 September 8, 2003: Steady-State with Homogeneous Chemical Reaction

Mechanics:

- New recitations: R12, F2, both in 8-306.
- Fri: very different lecture, ABET stuff.

Names.
Muddy stuff:

- Recitations. :-)
- Dislike cgs units.
- Clearer writing and neater presentation. (Big chalk...)
- Why both ways? One is simple but wrong, other is complex and right.
- Flux in cylindrical coordinates. Give full gradient. (Next time.)
- Integrating to get solution: $d/dr(rdC/dr) = 0 \Rightarrow C = A' \ln r + B$.
- General⟶particular solution in cylindrical coords. Start with general, plug in BCs:

$$C = A \ln r + B \tag{2.19}$$

$$\begin{aligned}
C_{in} &= A' \ln R_1 + B && (2.20)\\
C_{out} &= A' \ln R_2 + B && (2.21)\\
C_{out} - C_{in} &= A'(\ln R_2 - \ln R_1) && (2.22)\\
A' &= \frac{C_{out} - C_{in}}{\ln(R_2/R_1)} && (2.23)\\
C_{in} &= \frac{C_{out} - C_{in}}{\ln(R_2/R_1)} \ln R_1 + B && (2.24)\\
B &= C_{in} - \frac{C_{out} - C_{in}}{\ln(R_2/R_1)} \ln R_1 && (2.25)\\
C &= \frac{C_{out} - C_{in}}{\ln(R_2/R_1)} \ln r + C_{in} - \frac{C_{out} - C_{in}}{\ln(R_2/R_1)} \ln R_1 && (2.26)\\
C - C_{in} &= \frac{C_{out} - C_{in}}{\ln(R_2/R_1)} \ln(r/R_1) && (2.27)\\
\frac{C - C_{in}}{C_{out} - C_{in}} &= \frac{\ln(r/R_1)}{\ln(R_1/R_2)} && (2.28)
\end{aligned}$$

- Didn't finish: timescale to steady-state $\tau \sim L^2/D$, in this case 125,000 seconds, about a day and a half. Will explore this more rigorously on Friday.

Summarize: illustrates 3.185 methodology

- Problem statement: maximize throughput = flux×area
- Conservation equation
- Constitutive equation
- Combine to give (partial) differential equation

- General solution with integration constants
- Boundary conditions give values of integration constants
- Use solution to get problem objective: flux×area
- Design recommendation follows from solution

Like p. 465 of W^{3}R.

Generation Homogeneous chemical reactions. RCC carbon fiber-reinforced graphite composite! Very high-temperature, high-strength. Carbon fiber preform, model as a porous material, diffusion of acetylene to the surfaces of the fibers, at high temp it decomposes and deposits graphite.
Problem: as it deposits, it seals off the entrances, non-constant diffusivity. Generation of acetylene $G = -kC$. UNITS!
Set up problem in center, symmetry, sheet of material. 1-D equation:

$$0 = D\frac{d^2C}{dx2} + G = D\frac{d^2C}{dx^2} - kC \tag{2.29}$$

General solution, using polynomials e^{Rx}, $R = \pm\sqrt{k/D}$, so

$$C = A\exp\left(x\sqrt{\frac{k}{D}}\right) + B\exp\left(-x\sqrt{\frac{k}{D}}\right) \tag{2.30}$$

BCs: at $x = \pm\frac{L}{2}$, $C = C_0$, so $A = B$,

$$C_0 = A\left[\exp\left(\frac{L}{2}\sqrt{\frac{k}{D}}\right) + \exp\left(-\frac{L}{2}\sqrt{\frac{k}{D}}\right)\right] = A\cosh\left(\frac{L}{2}\sqrt{\frac{k}{D}}\right) \tag{2.31}$$

Result:

$$\frac{C}{C_0} = \frac{\cosh\left(x\sqrt{\frac{k}{D}}\right)}{\cosh\left(\frac{L}{2}\sqrt{\frac{k}{D}}\right)} \tag{2.32}$$

What does this look like? Pay attention to $\frac{L}{2}\sqrt{\frac{k}{D}}$, or more generally, $\frac{L^2k}{D}$. Can either be sorta uniform, or VERY non-uniform, uniform if that number is small (thin sheet, slow reaction, fast diffusion), nonuniform if it's large (thick sheet, fast reaction, slow diffusion). Makes sense.

So, have process, want to double thickness with same uniformity, can't change D much, how much change k? Drop by factor of 4. Problem: takes four times as long!!

The real solution: blow acetylene through it!

2.3 September 10, 2003: Unsteady-State Diffusion

TODO:

- Check reading room to make sure texts are there.
- Bring: cards, class list.
- Check W^3R pages for this lecture.

NAMES!
Mechanics:

- Get office hours together.
- Pump the zephyr instance.
- Fri: very different lecture, ABET stuff.

Muddy stuff:

- Cylindrical gradient (W^3R appendices A-B, p. 695–700):

$$\nabla C = \frac{\partial C}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial C}{\partial \theta}\hat{\theta} + \frac{dC}{dz}\hat{z}, \tag{2.33}$$

$$\begin{aligned}\nabla^2 C &= \frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{1}{r^2}\frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2}, \text{ or} && (2.34)\\ &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2}, \text{ or} && (2.35)\\ & && (2.36)\end{aligned}$$

- During derivations, important points are obscured. "What we've learned" summaries help. Basically following outline mentioned before, on p. 465 of W^3R. Also feel free to snooop around Athena directory...
- How to draw exponentials in concentration profile?
- Plotting hyperbolic trig functions—necessary? No. If needed, use calc/table.
- Too quick jump from integ consts to carbon fiber material, missed lots.
- Keep C_2H_2 conc constant for constant rate? Not quite, keep it uniform.
- How to calculate C_2H_2 consumption rate? Use concentration (or partial pressure) and reaction constant. But often don't know reaction constant, need to try at various temperatures, or just do what we did—find something which works, and use this methodology to understand why and how to make work for new designs.
- How do we get:

$$\lim_{\Delta x \to 0} -D\frac{\frac{dC}{dx}\big|_x - \frac{dC}{dx}\big|_{x+\Delta x}}{\Delta x} + G = D\frac{d^2C}{dx^2} + G? \tag{2.37}$$

  Derivative of the derivative is the second derivative?

- Arrhenius plot: which part is diffusion-limited, which part reaction-limited? Can't really compare because of different units. But can sort of make a plot of $\log(kL^2/D)$ vs. $1/T$, look at different parts. Want: low-temperature reaction-limited case, with fast diffusion to wipe out conc gradients. Diffusion-limited means it doesn't diffuse in very far.

  Next Monday: reaction and diffusion in series, which dominates is more straightforward, can easily compare the different coefficient.

- How did $\sqrt{k/D}L/2$ become kL^2/D? What's important for design: if two designs have the same kL^2/D, then have the same $\sqrt{k/D}L/2$, same uniformity. So use the simpler one to guide design decisions. Get into further with dimensional analysis next week.
- Why no flux at $x = 0$? Because of symmetry: on left, flux goes right; on right, flux goes left; in middle, flux goes... nowhere! Symmetry, or zero-flux boundary condition, like PS2 #3.

Unsteady Diffusion Last two times: stories to take home: increasing production rate of helium from natural gas, high-quality manufacturing of reinforced carbon-carbon for space shuttle wing, nose leading-edge tiles. This time: math first, examples later, because three different solutions to the diffusion equation, examples can use one or more.

Now accumulation != 0, rate also in mol/sec = $V\partial C/\partial t$. Chapter 27 material. Resulting equation in 1-D:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} + G. \tag{2.38}$$

Physical intuition: concentration curvature is either due to generation, or leads to time evolution, or both. Upward curvature means neighbors diffuse in, either G negative or C increases; downward means diffuse out, either G positive or C decreases.

Today focus on zero-generation solutions which you've seen before, to be used in this class (book derives them using Laplace transforms...):

- Error function:

$$\begin{aligned}
C &= A\text{erf(c)}\left(\frac{x}{2\sqrt{Dt}}\right) + B, &(2.39)\\
\frac{\partial C}{\partial t} &= -\frac{x}{2\sqrt{\pi D t^3}}\exp\left(-\frac{x^2}{4DT}\right), &(2.40)\\
\frac{\partial C}{\partial x} &= \frac{2}{\sqrt{\pi}}\frac{1}{2\sqrt{Dt}}\exp\left(-\frac{x^2}{4DT}\right), &(2.41)\\
\frac{\partial^2 C}{\partial x^2} &= -\frac{1}{\sqrt{\pi D t}}\frac{2x}{4Dt}\exp\left(-\frac{x^2}{4DT}\right) &(2.42)\\
&= -\frac{x}{2\sqrt{\pi D^3 t^3}}\exp\left(-\frac{x^2}{4DT}\right). &(2.43)
\end{aligned}$$

So this satisfies equation 2.38.

What it looks like: graph erf, erfc; discuss constant C BC $x = 0 \Rightarrow C = C_0$, uniform C IC $t = 0 \Rightarrow C = C_i$. Results:

$$C_i > C_s \Rightarrow C = C_s + (C_i - C_s)\text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{2.44}$$

$$C_s > C_i \Rightarrow C = C_i + (C_s - C_i)\text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{2.45}$$

Semi-infinite. But what if your part is not semi-infinite, but thickness L? (Not many parts are semi-infinite...) Since erf(2)=0.995 and erfc(2)=0.005, we can approximate $\infty \simeq 2$, if $\frac{L}{2\sqrt{Dt}} > 2$, then erf is about 1 and erfc about 0, can consider semi-infinite. Solve for t:

$$t < \frac{L^2}{16D} \Rightarrow \text{semi} - \text{infinite}. \tag{2.46}$$

(Recall $t > L^2/D \Rightarrow$ steady-state...)

- "Shrinking Gaussian":

$$C = \frac{A\delta}{\sqrt{\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) + B \tag{2.47}$$

$$\frac{\partial C}{\partial t} = ... \tag{2.48}$$

Graph: initial layer of height $A + B$ in background of B, spreads out. Note: not valid for short times, only for

$$2\sqrt{Dt} > \delta \Rightarrow t > \frac{\delta^2}{4D}. \tag{2.49}$$

Note also (semi-)infinite, like erf valid for $t < L^2/16D$. Note one-sided, two-sided; either way, BC at $x = 0 \Rightarrow \partial C/\partial x = 0$.

Not necessarily square initial condition! Can even start with erf, drive in to shr Gaussian.

2.4 September 12, 2003: 9/11 remembered, ABET

TODO: Bring ABET handout!
Schedule office hours.

September 11. The day meant a lot of things to a lot of people. Yesterday the occasion was commemorated in a number of ways, here in Boston, in my hometown of New York City, and around the country and the world. I can't hope to be as profound as some of the speakers at those services, but can talk about a few things it meant to me personally, in particular as I have reflected on my decision to become an engineer, and my purpose in the profession. Perhaps some of it will resonate with one or two of you; I invite your comments or questions, and we'll take as long for this as we have to.

I'd like to start nine days before the tragedy, when I was in New York for my sister-in-law's wedding. My wife's parents live in Brooklyn, which is where the ceremony was held, but we were staying with her aunt and uncle in Long Island. At least twice a day in the few days beforehand, we drove the Belt Parkway and Brooklyn-Queens Expressway, wrapping around Brooklyn, passing under the Verazzano bridge and entering New York Harbor, with the view of the Statue of Liberty and the majestic buildings rising ahead, the skyline dominated, of course, by the World Trade Center.

During those drives, I recalled the experience of my High School French teacher Mr. Schwartzbart, an Austrian Jew who survived World War II in a rural Belgian boys' camp which, unknown to him at the time, was made up entirely of Jewish boys, and in fact, was set up to keep them safe throughout the Nazi occupation. He described the terror he felt under the occupation, and then the arrival of the American soldiers, "All of them giants," he said, then pointed to me, "like Adam," they had come to set the continent free.

And he described the journey to America as a young teenager, a transforming experience. Most amazing was the entry of his ship carrying scores of poor immigrants like himself into New York Harbor, this impossibly enormous bridge which just got bigger and bigger as they approached (the Verazzano was the longest span in the world for about 50 years), the tranquility of the harbor within, with the great buildings visible ahead including the Empire State, and the Statue of Liberty to his left as they steamed toward Ellis Island (the World Trade Center's construction was still 20 years away). There was an awe-inspiring sense of the magnitude of this great nation of impossible size which had overwhelmed some of the greatest evil the world had ever known, and his heart swelled with joy at the thought that there was such power on the side of liberty.

These days in is fashionable to reflexively cringe at the identification of this country with freedom, and this teacher in particular very frequently commented cynically on the deficiencies in American culture and education. Having come to know this side of him, when we asked why he came to this country, Mr. Schwartzbart's reply surprised us: "The land of the free and the home of the brave." Then after a pause, "It really is true." His personal experience of this gave great weight to these words.

During these drives along the Belt Parkway, my thoughts also turned toward the fragility of the grand edifices, and in particular to the 1993 bombing of the underground parking lot of one of the Twin Towers. Fortunately the towers withstood that attempt to destroy them, but there would surely be more attempts, and no amount of devastation was too horrible for the perpetrators to dream up. Should anything happen, I was grateful for the opportunity to see this beauty, and even to feel a small piece of what Paul Schwartzbart had felt some fifty years earlier. I thought of how fortunate is his generation which came through the Depression, fought that terrible war, and lived to see the nation preside over such a long and prosperous peacetime as the world had perhaps never before known.

So you can imagine my shock when just nine days later, as I sat in my office, my wife called from home to say that while watching CNN, they announced that a plane had crashed into the World Trade Center. Well, I thought, about 60 years ago a small plane hit the Empire State building, I'm sure there was a lot of damage and many people killed, but the rest of the building should be fine. Just a few minutes later she called again to tell me about the second plane, and suddenly I was afraid. Then the Pentagon, and the missing plane in Pennsylvania. My thoughts turned to the Mid-East, and this administration's policy of deliberate neglect in the Israeli-Palestinian peace process. Then the last call, one tower had collapsed. With her voice choking from the tears, she described its fall as "like a house of cards," and could say little more.

Immediately, I logged out, got on my bike, and pedaled home as fast as I could.

I'm sure each of us can tell a story about where we were when it happened. Being from New York, I was immediately concerned for friends and family. My wife's grandmother went to the roof of her building in Queens, from where she saw the second plane hit the south tower, and that tower's collapse. I had shared this view every day growing up as I rode the Roosevelt Island tramway to school and saw these buildings which seemed as permanent as mountains. My wife's best friend in College, who lives in the Prospect Heights section of Brooklyn and works in the southern tip of Manhattan, noticed people in his neighborhood looking up and saw some smoke, but rushed into the subway as he was late for work; the packed subway stopped after it left Brooklyn and waited in the tunnel for about 20 minutes before it turned back and he got out and learned what had happened. My Elementary School best friend worked in the 17th floor of Tower 1, and had a bad back which would have made it painful and difficult to get out—if he hadn't been home sick that day.

Then there was my father's friend whom I know well and whose business had just finished moving into the 89th floor of Tower 1. His staff had been told not to come in that morning until 10 AM, because their carpets, freshly washed during the 1-7 AM shift, would need to finish drying. As he drove north on the New Jersey Turnpike, he saw the first plane crash right through the windows of his new office, then took the next exit and went right back to his daughter's kindergarten class.

The previous Spring and Summer I had a course 6 UROP student in my group. His brother worked above the 90th floor of Tower 2, and on the first and second day afterward without a word to anyone in his family, my student grew panicked, then desparate, then increasingly hopeless. His brother finally called to say that a friend had literally dragged him from the office after the first plane hit, and they ran out of the building together just as the second plane smashed into it. He described bits of the hell that was the area around him, but at the time had no other thought than to get away, go home and lie down in shock, not even thinking about his relatives who were trying to reach him. My student described the moment when they connected as one of the happiest of his life.

Another friend was not so fortunate. Her father worked in an upper floor of Tower 2, and was one of just two in his company who didn't make it out. To make matters worse, she was trapped in L.A. because of grounded planes, unable to get back and try to locate him, so day upon day she was not only uncertain and hurting but frustrated at being far from anyone who could help her. She is still grieving, as it's hard to accept that she lost the closest person to her in the world because a handful of maniacs decided to crash a plane into his building.

There are of course tens of thousands more stories like these, so many people were affected directly or knew someone who was. But even if you were not so directly involved, if you're like me, the tragedy didn't end on that day, but played out over and over again in your mind. I can't count how many mornings in the ensuing months I woke up at 3 AM thinking about the towers' collapse, feeling hurt, afraid, angry, and much as I hate to admit it, somewhat vindictive as we learned of the total destruction of the Al Queda camps and cave complexes in Afghanistan.

Then thoughts turned to my own life. What can I do, what's my role in the world, how can I help?

I turned to the motivations I had for entering science and engineering, and materials science in particular, which I came up with in High School. Motivations for studying these things vary greatly, from interest in the subject matter, elegance of the equations, beauty of nature etc., to being able to earn a stable income and support a household, or perhaps a large income, to serving society in some way. My own motivations fell somewhat in the first category, but if I had followed that alone I would have been 6-3 (computer science); it was the last of these categories, serving society, which steered me into Materials Science.

As a high school student, I verbalized this service as follows. As a scientist or engineer, I would be helping to solve the world's little problems, which I listed as:

- Agriculture, to feed a growing planet.
- Medicine, allowing people to lead longer, healthier lives.
- Transportation and communications, to bring people together and lessen the chances of conflict. For example, much of the reason war between France and Germany today is unthinkable is because there are so many more personal cross-border relationships now than in 1940 or 1914, it's very difficult for a propagandist to castigate an entire people as "the enemy" and it's becoming more difficult every year.

- Human interactions with the environment, for sustainable living.
- A recent addition, information access, with implications for democracy, as the biggest enemy of an authoritarian state is the truth.

All of these are important in themselves, but even more important, if we do our jobs well and make a difference in these areas, we help the artists, politicians, economists, philosophers and theologians to solve the big problems, which I would list as:

- World peace.
- Averting famines, and their relief. Almost all famines can be avoided without resort to international aid, and are the result of poor resource management or hoarding.
- Real public health, made available to those who need it around the world.
- Justice, including somewhat equitable economic distribution.
- Truth in journalism and history.
- Human happiness and fulfillment.
- Purpose and meaning for our lives.
- Artistic expression of emotions, of values, of that purpose and meaning.
- Last year Ross Benson added: Tolerance of differences.

An important consequence of this understanding of “little problems” and “big problems” is that being a scientist or engineer requires a lot of *faith*, faith that our knowledge and our inventions will be used wisely, for good and not for evil. The more “sciencey” our contributions, the more faith is necessary, with the ultimate example perhaps being nuclear science, which can be used to produce lots of cheap power or cure diseases, or destroy entire cities in an instant. If we work on weapons, they can of course be used for defense or for aggression.

But even if we’re not working on nuclear science or weaponry, one of the lessons of September 11 for me is that no matter how careful we are to focus on purely non-military technologies, this tragedy showed that even a civilian jetliner—built to bring people together—can be abused by people with sufficient hatred as a weapon of mass destruction. This is truly frightening for us, and requires us to have that much more faith in the people, institutions and systems surrounding the technology in whose development we participate.

So what should we do? Shall we abandon technology altogether and go back to rubbing sticks together? Perhaps we should join the peace corps? For some of us that will be the answer, but I think there’s a lot more that can be done with the little problems that can help to make a real impact on the big ones. So how can we put ourselves in positions to do as much good as possible?

I can think of a few ways, but at your age and even at mine, perhaps the most important is to take a step back and examine what we’re doing and why. I have an advisee taking this class now who took off all of last Spring for that very purpose, and ended up returning to MIT (and in fact to Materials Science) that much more focused than the previous December for the experience. Of course, you don’t have to take off a semester to do this, there are very good ways to do some of this right here.

First, the HASS and HASS-D subjects present outstanding opportunities for this kind of exploration. MIT is no longer just about training technology leaders, but also about training world leaders who know about technology, and this school has put enormous resources into building world class departments in the Humanities, Arts and Social Sciences. For example, I’ve heard tremendous things about our Anthropology department from a variety of external sources, and even within our department we offer a HASS subject called Materials in the Human Experience (3.094) every Spring.

Second, I’ve made a point of suggesting to all of my advisees that they get to know the MISTI programs (I think that stands for MIT Internships in Science, Technology and Industry), which do an outstanding job not just of sending students to companies, universities and government labs in foreign countries, but also preparing them for the trip, even culturally and psychologically.

Third, develop a habit of using your wealth to support organizations and causes which effectively promote what you view as positive values. You may not have much now, but you will later, and getting into this habit is not hard; furthermore, membership in many of these organizations requires a contribution of as little as $30. If you like I can discuss offline some of the organizations I've given to since my undergraduate years, one even since high school.

Fourth, look for opportunities to participate in the process of improving lives yourselves. Whether tutoring or mentoring, or working in a social justice organization, or writing to Congress, participating in society in a meaningful way is important to making it all work, and I believe important to improving ourselves too. Believe it or not, time is actually one resource which you will *not* have more of later in life than you have now, particularly if children become part of your life.

Fifth and perhaps most importantly, get to know your fellow students. This buzzword is repeated over and over again, but it's worth repeating yet again: because MIT attracts the best and brightest from all over the world, the *diversity* of the students on this campus is truly extraordinary, it's almost certainly broader and deeper than anything you've experienced before college, and almost certainly broader and deeper than anything you will ever experience later in life. That goes for Cambridge as well, and many other universities, though much less so on the graduate level and beyond. And by getting to know your colleagues, I don't just mean hanging out and eating pizza, nor even getting to know what spices they use to cook lamb, though food is of course an important part of social interaction. I'd encourage you to learn something about your friends' lives, their families, their values—and be willing to discuss these aspects of yourselves too.

And given its importance, I'd encourage you to learn something about your friends' faith. Human institutions, organizations, systems and even nations are terrific, but never perfect, as we learned in a powerful way on September 11. Participating in and strengthening them is an important and honorable activity, but I believe that placing all of our hope on them is not viable in the long term. At some point they're going to let us down, as this country has in some ways let down my French teacher Mr. Schwartzbart. Furthermore, evidence abounds for forces at work in the universe beyond those of physics, and even grows with the increase of human knowledge about this universe; perhaps the most significant example is the Anthropic Principle in Cosmology, which some of you may have heard of and I'd be happy to discuss offline.

That concludes what I said last year: the tragedy reminds us that our work here is very important, but must be viewed in context, and done with faith that it will be used for the broad purposes for which we intend it. Since last year, time has passed and some of the emotions have subsided just a bit, also several important things have happened, or have not happened, causing my own feelings about this to be somewhat more complicated.

For one thing, the message from Washington continues to urge us to live out lives as if nothing had happened, because if we changed anything, we'd be giving the terrorists what they want. But this is foolishness, important things have changed, and as citizens there are things we can do on a daily basis to improve our country's security, and the silence from Washington has been deafening.

A few months ago I saw a book provocatively titled, "When you ride alone, you ride with bin Laden." The cover art was derived from a World War II poster, "When you ride alone, you ride with Hitler," whose point was that the practices of avoiding driving, carpooling, and using public transportation save gasoline needed for the war effort. In that vein, an important thing which has *not* happened is that there has been no effort whatsoever on a national level to reduce our dependence on imported oil, which has been a huge factor in our problems in the Middle East. In fact, we've seen the opposite in this administration's rollback in fuel economy standards, and heard talk about the costs to the auto manufacturers and consumers of requiring increases in efficiency, with no mention whatsoever of the multitude of costs of continuing to burn fossil fuels as extravegantly as we like.

Another thing which has changed my view of the world was the war in Iraq. For months, the administration hyped any evidence at all for Iraqi connections to Al Qaeda and possession or development of weapons of mass destruction. Then inspections were allowed (to be fair, largely due to U.S. pressure, and no thanks to the posturing of certain countries like France), and one-by-one the inspections eliminated every piece of purported WMD evidence save the rumor about uranium purchase from Niger. And so with that one rumor as justification, we sent an invasion force to Kuwait, and used technological superiority to destroy the Iraqi army in about four weeks.

I believe that the war was wrong for a number of reasons. First, as mentioned, it was completely unjustified. There was no correlation to terrorism, none to weapons of mass destruction, and there are a dozen dictators around the world whose human rights violations could similarly motivate action. If violation of U.N. resolutions was the motive, then it's up to the U.N. to act.

Second, this war was an extremely imprudent waste of resources. It is unwise to spend a couple of hundred billion dollars on a flimsily-justified war in a time of record deficits, and even more imprudent to tie down fifteen of the U.S. Army's thirty-three combat brigades in that occupation during a time of multiple threats from WMD in North Korea and Iran, to shaky stability in Afghanistan, to low-level al Qaeda activity from Indonesia to Somalia. And most significant is the loss of hundreds of American and thousands of Iraqi lives, very nearly including that of my own brother, a Captain in the U.S. Army third infantry division's second brigade, whose unit was hit by an Iraqi missile just after their capture of downtown Baghdad. Like my Course 6 UROP student two years ago, the days between learning of the attack and confirming my brother's safety were some of the longest of my life. I cannot imagine the terror and grief of hundreds of thousands of loved ones of Iraqi soldiers who did not know for weeks or months whether their sons, brothers, husbands or fathers were dead or alive, nor the pain of those whose worst fears were in the end confirmed.

Finally, the war has cost us diplomatically, and will continue to cost us potentially for many generations. The arrogance with which the administration shrugged off overwhelming international opposition was shocking, prticularly as it involved three of the five Security Council permanent members, some of our most important allies, and both of our neighbors. Even more shocking was the pathetically childish pettiness with which the administration spoke of "punishing" the opponents to the war—particularly the French—and then turned around to ask them to contribute money and troops to the occupation and reconstruction to reduce the resource burden on us. But in the long term, the most diplomatically destructive aspect of the war is the precedent it sets for accusing a nation of violations of one sort or another, putting aside international outcry for restraint, and using military superiority to crush the weaker victim. This precedent can easily be abused by, say, Turkey, Syria, Egypt, Jordan and Saudi Arabia against Israel, North Korea against the South, Russia against the former Soviet Republics, China against Taiwan—any nation with a fight to pick can say, "But of course it's been done before, by the Land of the Free and Home of the Brave!"

And so we are reminded of our duty as citizens to speak out about matters of importance to our country. And in particular, as scientists and engineers we have the duty to speak out with authority on certain issues such as the small cost of reducing energy consumption, and the enormous costs of not doing so. Most of all, in the changed world our need for faith is greater than ever, in our work as well as our outlook for the future. I welcome any comments, contributions, or questions.

ABET Sheet Review See the ABET sheet.

Unsteady Diffusion Continued Muddy stuff:

- Symbol conventions: C_i is initial, C_0 I use as surface and sometimes other things; C_s always surface concentration.
- Physical meaning of graphs, interpretation of these things: coming soon.
- Exact criteria for each solution: will be summarized.
- Semi-infinite and erf validity. First, semi-infinite applies to one-sided erf and one-sided shrinking Gaussian. Fully infinite applies to two-sided both. Second, the criterion is derived from the error function: $t < L^2/16D \Rightarrow \text{erf}(x/2\sqrt{Dt}) > 0.995$ and erfc is below 0.005. Same criterion for erf, erfc, shrinking Gaussian.
- How do the M and top-hat initial conditions give the same equation? Over a long time, the details of the initial condition smooth out and become Gaussian.

Continuing where we left off last time (did the erf and shrinking Gaussian):

- Fourier Series:

$$C = a\exp(-b^2Dt)\sin(bx)(\text{or } \cos), \tag{2.50}$$

$$\frac{\partial C}{\partial t} = -ab^2 D \exp(-b^2 Dt) \sin(bx), \tag{2.51}$$

$$\frac{\partial C}{\partial x} = ab \exp(-b^2 Dt) \cos(bx), \tag{2.52}$$

$$\frac{\partial^2 C}{\partial x^2} = -ab^2 \exp(-b^2 Dt) \sin(bx). \tag{2.53}$$

$$\tag{2.54}$$

Elegant and simple. Separation of variables: all of the t in one term, all of the x in the other $f(t)g(x)$. [Eigenfunctions...]

Graph: sine wave decays with time.

2.5 September 15, 2003: Wrapup unsteady, boundary conditions

Muddy from last time:

- Appreciate 9/11 reflections, not political opinions. Apologies to those affected, particularly language. Forms a strong part of 9/11 feelings, particularly as administration has done its best to tie them together. Uncomfortable with talking about one side and not the other. War must always be a last resort when other means e.g. negotiation have been tried. Defining objectives as narrowly as “regime change” with neither aggression nor clear and present danger (Bush *and* Clinton) is as misguided and wrong as extremists in the region who call for destrurction of a certain state “by any means necessary”. Open for last words...

Continuing where we left off last time (did the erf and shrinking Gaussian):

- Fourier Series:

$$\begin{aligned} C &= a\exp(-b^2Dt)\sin(bx)(\text{or } \cos), && (2.55)\\ \frac{\partial C}{\partial t} &= -ab^2D\exp(-b^2Dt)\sin(bx), && (2.56)\\ \frac{\partial C}{\partial x} &= ab\exp(-b^2Dt)\cos(bx), && (2.57)\\ \frac{\partial^2 C}{\partial x^2} &= -ab^2\exp(-b^2Dt)\sin(bx). && (2.58)\\ & && (2.59)\end{aligned}$$

  Elegant and simple. Separation of variables: all of the t in one term, all of the x in the other $f(t)g(x)$. [Eigenfunctions...]

  Graph: sine wave decays with time. Like a sinusoidal layered material being annealed in time. If period=$2L$, then $b = \pi/L$, get:

$$C = a\exp\left(-\frac{\pi^2Dt}{L^2}\right)\sin\left(\frac{\pi x}{L}\right). \tag{2.60}$$

  But what use is a sine wave? Note linearity of diffusion equation: any sum of solutions is also a solution. So we can add sine waves to get something more useful, use that.

  Fourier transform: express *any* initial condition as sum of sine waves. We’ll do one: square wave of period $2L$ for multilayer material annealing, each term has period $2L/n$ so $b_n = n\pi/L$:

$$C = \sum_{n=0}^{\infty} a_n\exp\left(-\frac{n^2\pi^2Dt}{L^2}\right)\sin\left(\frac{n\pi x}{L}\right). \tag{2.61}$$

  The Fourier transform:

$$a_n = \frac{4}{n\pi},\ n \text{ odd},\ 0,\ n \text{ even}. \tag{2.62}$$

  Illustrate different sine functions, how they add to a square wave. Result:

$$C = C_0 + (C_{max} - C_0)\sum_{n=1, n \text{ odd}}^{\infty} \frac{4}{n\pi}\exp\left(-\frac{n^2\pi^2Dt}{L^2}\right)\sin\left(\frac{n\pi x}{L}\right). \tag{2.63}$$

  So we start with all these sine waves, then what happens? Higher-order terms shrink real fast. Graph amplitude vs. time, show $n = 3$ drops out nine times faster, $n = 5$ twenty-five times faster. Do it as t/τ, where $\tau = L^2/\pi^2D$, so first term is $\exp(-t/\tau)$, second $\exp(-9t/\tau)$. One term remains real fast.

  Consider: $t = L^2/D$... What is single-term max concentration at that time? $4/\pi \times \exp(-\pi^2) = 6.5 \times 10^{-5}$, quite close to zero!

Other application: finite system with thickness L, uniform IC, constant C boundary conditions. Graph, show the "virtual" wave outside. Note that at short times, erf is easier; long times, one-term sine wave is easy.

TA wanted to do 2-D and 3-D separation $C = f(t)g(x)h(y)$...

Suppose something more like first lecture, section 2.1 (p. 6): initial flat, one side raised? Then linear plus Fourier series, with odd and even n; even so, at $t = L^2/D$, first term, max conc is a tiny fraction of original. So, very close to steady-state!

Which to use? Summary of criteria:

- Error functions erf, erfc:
  - (Semi-)infinite
  - Uniform initial condition at $t = 0$ equal to boundary condition at $x = \infty$
  - Constant concentration boundary condition at $x = 0$, infinite source/sink backing it up.
- Shrinking Gaussian $\frac{A\delta}{\sqrt{\pi Dt}} e^{-x^2/4Dt} + B$:
  - (Semi-)infinite
  - Fixed amount of material already in solid and diffusing into infinity
  - Gaussian "width" $2\sqrt{Dt}$ much larger than δ
- Fourier series:
  - Infinite 1-D sine or square wave initial condition, *or*
  - Finite layer thickness L
  - Uniform initial condition at $t = 0$
  - Constant concentration boundary conditions at $x = 0$, $x = L$

Examples:

- Decarburizing steel sheet: initial concentration $t = 0 \Rightarrow C = C_i$, boundaries $x = 0, L \Rightarrow C = C_s = 0$ due to oxidation. Start erf, go to Fourier.
- Semiconductor devices: initial treatment with phosphorous-containing gas, initially no phosphorous so $t = 0 \Rightarrow C_P = 0$; fixed concentration at surface $C = C_eq$ or C_s or C_0. Erf. Then seal the top, no more gas, drive-in diffusion gives shrinking Gaussian.
- Galvanizing steel: thin layer of zinc on iron. Initial: $x < \delta \Rightarrow C = C_0$, $x > \delta \Rightarrow C = 0$. Start erf (diffusion couple) but centered at $x = \delta$

  $$C = \frac{C_0}{2} \operatorname{erfc}\left(\frac{x - \delta}{2\sqrt{Dt}}\right). \tag{2.64}$$

  This holds for as long as the zinc is semi-infinite, i.e. $t < \delta^2/16D$. For long times $t > \delta^2/D$, finite amount of zinc means shrinking Gaussian:

  $$C = \frac{C_0\delta}{\sqrt{\pi Dt}} \exp\left(-\frac{x}{4Dt}\right). \tag{2.65}$$

2.6 September 17, 2003: Boundary conditions, layer growth

Fun opener: Michael Dixon on calculus in physics in Dorchester.

Muddy from last time:

- Square wave: why is a_n zero for even n? That's the Fourier transform; would throw off symmetry.
- How erfs in infinite square wave IC? Like diffusion couple...
- What is plotted on the graph of amplitude vs. time?
- Steady Fourier: $\frac{4}{\pi}\exp(-\pi^2)$ constant? No, wave with that amplitude at $t = L^2/D$; for longer time asymptotically approaches $C = C_{av}$.
- In galvanizing situation, why erf for small times? Isn't it a finite amount of zinc? At very small times, can consider even the zinc as semi-infinite. Also, at small times $t < \delta^2/D$, shrinking Gaussian doesn't work, goes to infinitely tall and thin.
- What to use in example 3 between $\delta^2/16D < t < \delta^2/D$? Nothing covered here; perhaps another Fourier transform...
- Write down initial conditions for examples... Added to lecture notes, in my home directory.

Diffusion boundary conditions Types:

- Constant C: what's that C?
- Constant flux: sealed means zero, sometimes ion beams, etc. (not often)
- Flux vs. C, for chemical reaction or mass transfer coefficient. $J = k(C - C_{eq})$ (note ChemEs' k''...) Units: k in cm/s. Also mass transfer coefficient through fluid film: $J = h_D(C - C_{eq})$, where $h_D = \delta/D$.

Example: gas diffusion in metal. Oxygen, nitrogen, hydrogen in metals: diffuses monoatomically, $2\text{O(m)} \Leftrightarrow \text{O}_2\text{(g)}$, equation:

$$K_{eq} = \frac{p_{\text{O}_2}}{[O]^2}. \tag{2.66}$$

So oxygen concentration at equilibrium is proportional to the square root of pressure. (Not the same for helium, argon, etc.) Then if flux is proportional to difference in concentrations, it's proportional to square root of difference in partial pressures!

Misconception 1: Equilibrium is **NOT** steady-state. Global equilibrium here would be a brick of SiO_2. Local equilibrium gives concentrations at interface sometimes. Can be out of local equilibrium and at steady state too.

Misconception 2: kinetic reaction rate order is **NOT** thermodynamic order.

Layer growth Motivating example: silicon oxidation (example W^3R pp. 487-489). Electronic components, this is the "gate oxide" in MOSFETs, draw p-n-p structure. Thickness must be tightly controlled for the FET to work—to switch at the right voltage. How to make the oxide? Expose it to air, and it just grows. Cool. Wet oxidation too: expose it to steam and it grows differently (slower?). How much does it grow, how long to leave it there?

Go to the phase diagram, this one is pretty simple. Start with equilibrium. Many times, can use the phase diagram. Others, with impure phases (like air), or partial pressure or total pressure dependency, need activity to get equilibrium concentration at interface.

Out of equilibrium, but interfaces at local equilibrium: diffusion-limited, explain the concept of pseudo-steady-state. Growth is really slow because, although D might be high leading to steady-state, $C_3 - C_1$ is really small, leading to slow flux, really slow growth of the layer. Growth rate:

$$J_O = \frac{2 \text{ moles O}}{1 \text{ mole SiO}_2} \frac{\rho_{\text{SiO}_2}}{MW_{\text{SiO}_2}} \frac{dY}{dt}. \tag{2.67}$$

Why? Proportional to J_O, then it's just a matter of working out units.

No. $J\Delta t$ is the amount over a certain amount of time, $(C_1 - C_0)\Delta Y$ is the area on the graph needed to transform that much Si to SiO_2.

For equilibrium, set $J = \Delta C/Y$, solve for Y:

$$\begin{aligned}
\frac{C_3 - C_1}{Y} &= \frac{2 \text{ moles O}}{1 \text{ mole SiO}_2} \frac{\rho_{\mathrm{SiO}_2}}{M_{\mathrm{SiO}_2}} \frac{dY}{dt} && (2.68) \\
Y dY &= \frac{1 \text{ mole SiO}_2}{2 \text{ moles O}} \frac{M_{\mathrm{SiO}_2}(C_3 - C_1)}{\rho_{\mathrm{SiO}_2}} dt && (2.69) \\
\frac{Y^2 - Y_0^2}{2} &= \frac{1 \text{ mole SiO}_2}{2 \text{ moles O}} \frac{M_{\mathrm{SiO}_2}(C_3 - C_1)}{\rho_{\mathrm{SiO}_2}} (t - t_0). && (2.70)
\end{aligned}$$

Parabolic growth. Plotted in text, p. 489. But the plot doesn't quite work!

2.7 September 19, 2003: Layer Growth, Dimensional Analysis

Mechanics etc.

- Forgot last time: test 1 October 13?
- Monday: no class, but I will be here for office hours 2:30-3:30 as usual; Albert?
- Next Thurs 9/25: GE CEO Jeffrey Immelt at Bartos theater (downstairs Media Lab)...

Muddy from last time:

- Pseudo-steady-state of what? Diffusion: growth is slow, so conc profile reaches steady-state.
- Why $J_0 = \frac{\Delta Y}{\Delta t}(C_1 - C_0)$? Explain: $J_O \Delta t$ is the amount of oxygen which the flux has fed through. $(C_1 - C_0)\Delta Y$ is the amount of oxygen needed to transform ΔY worth of silicon into silicon dioxide.
- Why $Y(t)$? Is all diffusion-limited growth proportional to $\sqrt{t}$?

Layer growth Motivating example: silicon oxidation (example W^{3}R pp. 487-489). How much does it grow, how long to leave it there?

Back to phase diagram: C_0, C_1 and C_3 as three equilibrium concentrations at operating temperature. Out of equilibrium, but interfaces at local equilibrium: pseudo-steady-state.

For equilibrium, set $J = \Delta C/Y$, solve for Y:

$$\frac{Y^2 - Y_0^2}{2} = \frac{1 \text{ mole SiO}_2}{2 \text{ moles O}} \frac{M_{\text{SiO}_2}(C_3 - C_1)}{\rho_{\text{SiO}_2}}(t - t_0). \tag{2.71}$$

Parabolic growth. Plotted in text, p. 489. But the plot doesn't quite work!

Next out of local equilibrium: say 1st order chemical reaction as the slow step. (Note: kinetic order vs. thermodynamic equilibrium exponents!) Then introduce C_2 between C_1 and C_3, say the rate is proportional to $C_2 - C_1$, proportionality constant is the reaction rate coefficient which we call k. Very short times:

$$J = k(C_2 - C_1) \simeq k(C_3 - C_1),$$

constant growth rate, *linear* film growth.

Suppose C_3 at oxide outer surface, C_2 at back interface, C_1 in equilibrium with silicon, reaction limit with constant k, $J = k(C_2 - C_1)$. Want $J(C_3, C_1)$. Solve all together:

$$J = k(C_2 - C_1) = \frac{D}{Y}(C_3 - C_2) \left[\Rightarrow \frac{C_3 - C_2}{C_2 - C_1} = \frac{kY}{D}\right]$$

$$\left(k + \frac{D}{Y}\right) C_2 = kC_1 + \frac{D}{Y}C_3$$

$$C_2 = \frac{kC_1 + \frac{D}{Y}C_3}{k + \frac{D}{Y}} = \frac{\frac{kY}{D}C_1 + C_3}{\frac{kY}{D} + 1}$$

Now get J:

$$J = k\left(\frac{kC_1 + \frac{D}{Y}C_3}{k + \frac{D}{Y}} - C_1\right)$$

$$J = k\left(\frac{\frac{D}{Y}C_3 - \frac{D}{Y}C_1}{k + \frac{D}{Y}}\right)$$

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

Resistances in series. What dominates? Biot number! $\frac{kY}{D}$ Ratio of resistances. Small times and small Y mean small Biot, reaction-limited. Long times and large Y mean large Biot, diffusion-limited.

Dimensional analysis W^{3}R pp. 140–142. Definitions:

- Base units: m, s, mol
- Derived units: cm/s, N, mol/cm^3
- Dimensions: L, t, C_O

Step 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 the number of dimensions n, in this case $n = 5$.

This is done by intuition, and is very often the hardest step in the process.

Step 2 Find the number of base units in the system r. Here: cm, s, mol, so $r = 3$.

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

Step 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.

Counterexample: can't use k, D and Y because they're not independent! Very often there are multiple "right answers" (fluid dynamics), choose the one which is most convenient.

Step 5 Form the π groups from what's left, which are unitless versions of the parameters. Dimensionless J, called π_J, is $J \cdot [C_3 - C_1]^a \cdot [D]^b \cdot [Y]^c$. Easy way: make a table with base units across the top, start with dimensions of J. Which of the eliminated units have moles? $C_3 - C_1$, so we can say $a = -1$ and moles are cancelled. Then which have seconds? D, so we can say $b = -1$ and seconds are cancelled. Now there's just cm^{-1}, so $c = 1$ and we're done:

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

Likewise, π_k starts with k in m/s, so $a = 0$, $b = -1$, $c = 1$. Look, it's the mass transfer Biot number!

Step 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!

This ends diffusion, next week heat conduction!

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:

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

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

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

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: $\text{Bi}' = \frac{hV}{kA}$, $\text{Fo}' = \frac{\alpha A^2}{V^2}t$, 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:

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

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 $\frac{\text{W}}{\text{m}\cdot\text{K}}$. 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:

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

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

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

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 $\mathrm{Fo}_M > \frac{1}{2}$:

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

So, it's like a weighted average between $T_{i,n}$ and the average of the two (show graphically). When $\mathrm{Fo}_M > \frac{1}{2}$, 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:

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

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

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

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:

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

In 3-D:

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

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 $\alpha = 0.1 \frac{\mathrm{cm}^2}{\mathrm{s}}$, $u_x \sim 5 \frac{\mathrm{cm}}{\mathrm{min}} = \frac{1}{12} \frac{\mathrm{cm}}{s}$, 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.

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_BT (sketch molecules). Important thing is the Knudsen number, λ/L, given by:

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

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:

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

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: $\epsilon = f(T)$, $\alpha = f$(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 ⇒ resistance diagram!

New concept: zero-flux surface, well-insulated, reflected+emitted≃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!

Chapter 4

Fluid Dynamics

4.1 October 24, 2003: Intro, Newtonian Fluids

TODO: look up Wiedmann-Franz, falling film in new textbook.

Mechanics:

- PS5: Get the spreadsheet from the Stellar site (URL on PS was for PMMA properties).
- L expression may be off: calc'd to 7.9×10^{-9}, not 2.45×10^{-8}. Maybe a missing π.
- Subra on bionano cell mechanics next Monday 4PM 10-250. Recruiting...
- Next Tues: MPC Materials Day, on Biomed Mat'ls Apps. Register: http://mpc-web.mit.edu/

Muddy from last time

- First "rule" in viewfactor algebra: $A_1F_{12} = A_2F_{21}$, doesn't it depend on T? No, because F_{ij} is based only on geometry.
- F_{12} for facing coaxial disks with radii r_1 and r_2 sample graph: F_{12} is decreasing with d/r_1.

Fluid Dynamics! Brief introduction to rich topic, of which people spend lifetimes studying one small part. You will likely be confused at the end of this lecture, come to "get it" over the next two or three.

Categories: laminar, turbulent; tubes and channels; jets, wakes. Compressible, incompressible.

Outcomes: flow rates (define), drag force (integral of normal stress), mixing. Later couple with diffusion and heat conduction for convective heat and mass transfer.

Start: the 3.185 way. Momentum field, "momentum diffusion" tensor as shear stress. Show this using units: momentum per unit area per unit time:

$$\frac{\mathrm{kg}\frac{\mathrm{m}}{\mathrm{s}}}{\mathrm{m}^2 \cdot \mathrm{s}} = \frac{\mathrm{kg}}{\mathrm{m} \cdot \mathrm{s}^2} = \frac{\mathrm{N}}{\mathrm{m}^2}$$

Two parallel plates, fluid between, zero and constant velocity. x-momentum diffusing in z-direction, call it τ_{zx}, one component of 2nd-rank tensor. Some conservation of math:

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

Talking about momentum per unit time, $\frac{\mathrm{kg}}{\mathrm{m}\cdot\mathrm{s}^2}$, locally momentum per unit volume $\rho\vec{u}$. Here suppose u_x varies only in the z-direction, no τ_{xx} or τ_{yx}, no u_y or u_z. Three conservation equations for three components of momentum vector, here look at x-momentum:

$$V \cdot \frac{\partial(\rho u_x)}{\partial t} = A \cdot \tau_{zx}\big|_z - A \cdot \tau_{zx}\big|_{z+\Delta z} + V \cdot F_x$$

Do this balance on a thin layer between the plates:

$$W_x W_z \Delta z \frac{\partial(\rho u_x)}{\partial t} = W_x W_z \tau_{zx}\big|_z - W_x W_z \tau_{zx}\big|_{z+\Delta z} + W_x W_z \Delta z F_x$$

Cancel $W_x W_z$ and divide by Δz, let go to zero:

$$\frac{\partial(\rho u_x)}{\partial t} = -\frac{\partial \tau_{zx}}{\partial z} + F_x$$

What's generation? Body force per unit volume, like gravity. Units: $\mathrm{N/m^3}$ (like τ has N/m^2), e.g. ρg.

What's the constitutive equation for τ_{zx}? Newtonian fluid, proportional to velocity gradient:

$$\tau_{zx} = -\mu \left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right)$$

This defines viscosity μ, which is the momentum diffusivity. Units: $\mathrm{N \cdot s/m^2}$ or $\mathrm{kg/m \cdot s}$, Poiseuille. CGS units: $\mathrm{g/cm \cdot s}$, Poise = 0.1 Poiseuille. Water: .01 Poise = .001 Poiseuille.

So, sub constitutive equation in the conservation equation, with $u_y = 0$:

$$\frac{\partial(\rho u_x)}{\partial t} = -\frac{\partial}{\partial z} \left(-\mu \frac{\partial u_x}{\partial z} \right) + F_x$$

With constant ρ and μ:

$$\rho \frac{\partial u_x}{\partial t} = \mu \frac{\partial^2 u_x}{\partial z^2} + F_x$$

It's a diffusion equation!

So at steady state, with a bottom plate at rest and a top plate in motion in the x-direction at velocity U, we have: a linear profile, $u_x = Az + B$.

Aaliyah tribute: innovative complex beats, rhythmic singing, great performing. Started at an early age, passing at age 21? 22? a couple of years ago in plane crash was a major music tragedy.

4.2 October 27: Simple Newtonian Flows

Mechanics:

- Aaliyah: okay, you might have heard of her, but didn't expect from a Prof. MTV...
- Wiedmann-Franz: new text doesn't offer any help (p. 204, no constant).
- Subra on bionano cell mechanics next Monday 4PM 10-250. Recruiting...
- Tomorrow: MPC Materials Day, on Biomed Mat'ls Apps. Too late to register though :-(

Muddy from last time:

- Is the velocity in the x-direction, or the z-direction? x-direction, but it is quite confusing, τ_{zx} is flux of x-momentum in z-direction. Momentum is a vector, so we have *three* conservation equations: conservation of x-momentum, y-momentum, z-momentum. This vector field thing is a bit tricky, especially the vector gradient.
- I left out: a Newtonian fluid exhibits linear stress-strain rate behavior, proportional. Lots of nonlinear fluids, non-Newtonian; we'll get to later.

Intro: may be confused after last time. This time do a couple more examples with confined flow, including one cylindrical, hopefully clear some things up.

From last time: parallel plates, governing equation

$$\rho\frac{\partial u_x}{\partial t} = \mu\frac{\partial^2 u_x}{\partial z^2} + F_x$$

$$\frac{\partial u_x}{\partial t} = \nu\frac{\partial^2 u_x}{\partial z^2} + \frac{F_x}{\rho}$$

We have the diffusion equation! ν is the momentum diffusivity, like the thermal diffusivity $k/\rho c_p$ before it. Note: units of momentum diffusivity $\nu = \mu/\rho$: $\frac{\text{kg/m}\cdot\text{s}}{\text{kg/m}^3} = \text{m}^2\text{/s}$! Kinematic ($\nu$), dynamic ($\mu$) viscosities.

Note on graphics: velocities with arrows, flipping the graphs sideways to match orientation of the problem.

Cases:

- Steady-state, no generation, bottom velocity zero, top U:

  $$u_x = \frac{U}{L}z,\ \tau_{zx} = -\mu\frac{U}{L}$$

  Shear stress:

  $$\tau_{zx} = -\mu\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) = -\mu\frac{U}{z}$$

  Thus the drag force is this times the area of the plate.

- Unsteady, no generation, different velocities from $t = 0$.

  $$u_x = U\text{erfc}\left(\frac{L-z}{2\sqrt{\nu t}}\right), \tau_{zx} = -\frac{1}{2\sqrt{\nu t}}\frac{2}{\sqrt{\pi}}\exp\left(-\frac{(L-z)^2}{4\nu t}\right)$$

- New: steady-state, generation, like book's falling film in problem 4.15 of W^{3}R, with θ the inclination angle off-normal so $g_x = g\sin\theta$, z is the distance from the plane. The steady-state equation reduces to:

  $$0 = \mu\frac{\partial^2 u_x}{\partial z^2} + F_x$$

  $$u_x = -\frac{F_x z^2}{2\mu} + Az + B$$

BCs: zero velocity at bottom plate at $z = 0$, free surface with zero shear stress at $z = L$, $F_x = \rho g_x = \rho g \sin\theta$, result: B=0, get

$$u_x = \frac{g\sin\theta}{2\nu}(2Lz - z^2)$$

Shear stress:

$$\tau_{zx} = -\mu\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) = \rho g \sin\theta (L - z)$$

This is the weight of the fluid per unit area on top of this layer!

Shear stress as the mechanism of momentum flux, each layer pushes on the layer next to it. Think of it as momentum diffusion, not stress, and you'll get the sign right.

Flow rate: Q, volume per unit time through a surface. If width of the falling film is W, then flow rate is:

$$Q = \int_S \vec{u} \cdot \hat{n} dA = \int_{z=0}^{L} u_x W dz = \frac{Wg\sin\theta}{\nu}\left[\frac{Lz^2}{2} - \frac{z^3}{6}\right] = \frac{Wg\sin\theta}{\nu}\frac{L^3}{3}$$

Average velocity is Q/A, in this case Q/LW:

$$u_{av} = \frac{Q}{LW} = \frac{g\sin\theta L^2}{3\nu};$$

$$u_{max} = u_x|_{z=L} = \frac{g\sin\theta L^2}{2\nu}.$$

So average velocity is 2/3 of maximum for falling film, channel flow, etc.

4.3 October 29: 1-D Laminar Newtonian Wrapup, Summary

Mechanics:

- Next Weds 11/5: 3B Symposium!

Muddy from last time:

- Erf solution: why
$$u_x = U\text{erfc}\left(\frac{L-z}{2\sqrt{\nu t}}\right)?$$
  As long as it's semi-infinite, it's an erf/erfc solution (uniform initial condition, constant velocity boundary condition), so this works for $t \leq L^2/16\nu$. For erfs, they can start at 0, or somewhere else (zinc diffusion couple), and go "forward" or "backward". Graph the normal way. Also:
$$u_x = U\left[1 + \text{erf}\left(\frac{z-L}{2\sqrt{\nu t}}\right)\right]$$

- Weight of fluid: consider layer of fluid from z to L, it has force in x- and z-directions $F_g = V\rho g \sin\theta$ and $-\cos\theta$ respectively. In x-direction, shear goes the other way: $F_\tau = -\tau_{zx}A$. So force balance for steady-state (no acceleration):
$$V\rho g\sin\theta - A\tau_{zx} = 0 \Rightarrow \tau_{zx} = \frac{V}{A}\rho g\sin\theta = (L-z)\rho g\sin\theta.$$
  In z-direction, this is balanced by pressure:
$$P = P_{atm} + \rho g\cos\theta(L-z).$$

Nice segue into pressure-driven flows. Suppose fluid in a cylinder, a pipe for example of length L and radius R, P_1 on one end, P_2 on other. Net force: $(P_1-P_2)A_{xs}$, force per unit volume is $(P_1-P_2)V/A_{xs} = (P_1-P_2)/L$. Can shrink to shorter length, at a given point, force per unit volume is $\Delta P/\Delta z \to \partial P/\partial z$. This is the pressure generation term.

So, flow in tube: uniform generation throughout $(P_1 - P_2)/L$ (prove next week), diffusion out to $r = R$ where velocity is zero. Could do momentum balance, but is same as diffusion or heat conduction, laminar Newtonian result:
$$\rho\frac{\partial u_z}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial u_z}{\partial r}\right) + \rho g_z - \frac{\partial P}{\partial z}.$$
Here looking at steady-state, horizontal pipe, uniform generation means:
$$u_z = -\frac{F_z r^2}{4\mu} + A\ln r + B = -\frac{P_1-P_2}{4\mu L}r^2 + A\ln r + B.$$
Like reaction-diffusion in problem set 2 (PVC rod): non-infinite velocity at $r = 0$ means $A = 0$ (also symmetric), zero velocity at $r = R$ means:
$$u_z = \frac{P_1-P_2}{4\mu L}(R^2 - r^2).$$
What's the flow rate?
$$Q = \int_0^R u_z 2\pi r dr = \int_0^R \frac{P_1-P_2}{4\mu L}(R^2-r^2)2\pi r dr$$
$$Q = \frac{\pi(P_1-P_2)}{2\mu L}\left[\frac{R^2r^2}{2} - \frac{r^4}{4}\right]_0^R = \frac{\pi(P_1-P_2)R^4}{8\mu L}.$$
Hägen-Poisseuille equation, note 4th-power relation is extremely strong! 3/4" vs. 1/2" pipe...

Summary Summary of the three phenomena thus far:

	Diffusion	Heat conduction	Fluid flow
What's conserved?	Moles of each species	Joules of energy	momentum
Local density	C	$\rho c_p T$	$\rho\vec{u}$
Units of flux	$\frac{\text{mol}}{\text{m}^2\cdot\text{s}}$	$\frac{\text{W}}{\text{m}^2}$	$\frac{\text{kg}\frac{\text{m}}{\text{s}}}{\text{m}^2\cdot\text{s}} = \frac{\text{N}}{\text{m}^2}$
Conservation equation*	$\frac{\partial C}{\partial t} = -\nabla\cdot\vec{J} + G$	$\rho c_p \frac{\partial T}{\partial t} = -\nabla\cdot\vec{q} + \dot{q}$	$\frac{\partial(\rho\vec{u})}{\partial t} = -\nabla P - \nabla\cdot\tau + \vec{F}$
Constitutive equation	$\vec{J} = -D\nabla C$	$\vec{q} = -k\nabla T$	$\tau = -\eta\left[\nabla\vec{u} + (\nabla\vec{u})^T\right]$
Diffusivity	D	$\alpha = \frac{k}{\rho c_p}$	$\nu = \frac{\eta}{\rho}$

*Only considering diffusive fluxes. ^{T} in fluid constit. denotes the transpose of the matrix.

New stuff: vector field instead of scalar; very different units; pressure as well as flux/shear stress and force.

For those taking or having taken 3.11, shear stress τ relates to stress σ as follows:

$$\sigma = -\tau - PI$$

where p is $(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$, so $\tau_{xx} + \tau_{yy} + \tau_{zz} = 0$, $\tau_{xy} = \tau_{yx} = -\sigma_{xy} = -\sigma_{yx}$. Note that $\tau_{yx} = \tau_{xy}$ almost always, otherwise infinite rotation...

Also: mechanics uses displacement for $\vec{u}$, acceleration is its *second* derivative with time. Simple shear:

$$\rho\frac{\partial^2\vec{u}}{\partial t^2} = \nabla\cdot\sigma + \vec{F} \Rightarrow \rho\frac{\partial^2 u_x}{\partial t^2} = \frac{\partial\sigma_{xx}}{\partial x^2} + \frac{\partial\sigma_{yx}}{\partial y^2} + \frac{\partial\sigma_{zx}}{\partial z^2} + F_x = G\frac{\partial^2 u_x}{\partial z^2} + F_x.$$

Analogue to momentum diffusivity: G/ρ, units m^2/s^2, $\sqrt{G/\rho}$: speed of sound! Remember with a little jig:

Fluids are diffusive,
With their velocity and viscosity.
But on replacement with displacement,
it will behave, like a wave!

4.4 October 31: Mechanics Analogy Revisited, Reynolds Number, Rheology

Mechanics:

- Next Weds 11/5: 3B Symposium!
- 3.21 notes on Stellar (with η changed to μ).
- In all of the viewfactor problems of PS6, ignore the graphs dealing with "nonconducting but reradiating" surfaces in the text, as we didn't cover those this year (or last year).
- In disc graph, not r_1/r_2 but D/r_1 and r_2/D.
- In problem 2, "collar" refers to the heat shield, a cylinder above the ZrO2 source.
- In problem 3, the fluid layer is thin enough that we can neglect the curvature of the ram and cylinder. The ram motion is also vastly powerful in terms of driving flow than the weight of the fluid, so we can neglect rho*g in the fluid. With these two simplifications, velocity profile between the cylinder and ram is linear, making the problem a lot simpler.
- In problem 4a, Arrhenius means proportional to $\exp(-\Delta G_a/RT)$. For part b, think about what happens to glasses as they cool...
- In problem 5, think about conduction through a multi-layer wall, in terms of the interface condition. Also, just as the multi-layer wall has two layers with different values of A and B in the temperature graph T=Ax+B, here we have two fluid layers with different values of A and B in the falling film solution given in class (that solution is the answer to part a). The Reynolds number will be discussed in tomorrow's lecture.

Muddy from last time:

- Crossbar on z.
- Why is $A = 0$, $B = \frac{P_1-P_2}{4\mu L}R^2$ in tube? General solution:

  $$u_z = -\frac{P_1 - P_2}{4\mu L}r^2 + A\ln r + B,$$

  boundary conditions: $r = 0 \rightarrow u_z$ not infinite, $r = R \rightarrow u_z = 0$. So, nonzero A in $A\ln r$ gives infinite u_z at $r = 0$, use B to exactly cancel first term at $r = R$.

  Note: at axis of symmetry, $\partial u_z/\partial r = 0$, like temperature and conc; this too would give $A = 0$.
- Mechanics analogy: very rushed, deserves better treatment, even though not a part of this class.

Reynolds number Like other dimensionless numbers, a ratio, this time of convective/diffusive momentum transfer, a.k.a. inertial/viscous forces. Formula:

$$\text{Re} = \frac{\rho U L}{\eta}$$

Describes dimensionless velocity for dimensionless drag force f; also onset of turbulence.

- Tubes: $< 2100 \rightarrow$ laminar (very constrained).
- Channel, Couette: $< 1000 \rightarrow$ laminar.
- Falling film (inclined plane): $< 20 \rightarrow$ laminar, due to free surface.

Note didn't give number for turbulent, that's because it depends on entrance conditions.

Rheology Typical Newtonian viscosities:

- Water: $10^{-3}\mathrm{N \cdot s/m^2}$, density $10^3\mathrm{kg/m^3}$, kinematic viscosity (momentum diffusivity) $10^{-6}\mathrm{m^2/s}$.
- Molten iron: $5 \times 10^{-3}\mathrm{N \cdot s/m^2}$, density $7 \times 10^3\mathrm{kg/m^3}$, kinematic viscosity (momentum diffusivity) just under $10^{-6}\mathrm{m^2/s}$, close to water. Water modeling...
- Air: $10^{-5}\mathrm{N \cdot s/m^2}$, density $1.9\mathrm{kg/m^3}$, kinematic viscosity (momentum diffusivity) $5 \times 10^{-6}\mathrm{m^2/s}$, close to water!

But, very different effect on surroundings, drag force. So even though might flow similarly over a hill, geologists can tell the difference between water and wind erosion damage.

Liquids: generally inverse Arrhenius; gases (forgot).

Non-Newtonian: graphs of τ_{yx} vs. $\partial u_x/\partial y$. Categories:

- Dilatant (shear-thickening), example: fluid with high-aspect ratio solid bits; blood. More mixing, momentum mixing, acts like viscosity. Platelet diffusivity, concentration near walls...

  Model: power-law, $n > 1$.
- Pseudoplastic (shear-thinning), examples: heavily-loaded semi-solid, many polymers get oriented then shear more easily.

  Model: power law, $n < 1$.

  Next time: Wierd shear-thinning behavior at low strain rates due to fibrinogen content, extremely sensitive to fibrinogen and measures risk of cardiovascular disease better than smoking! (Gordon Lowe)
- Bingham plastic: finite yield stress, beyond that moves okay, but up to it nothing. Some heavily-loaded liquids, polymer composites, toothpaste; semi-solid metals bond together then break free.

  Model: yield stress τ_0, slope μ_P.

Power law relation:

$$\tau_{yx} = \mu_0 \left(\frac{\partial u_x}{\partial y} \right)^n$$

More than 1-D leads to wierd Tresca, von Mises criteria, etc.

4.5 November 3, 2003: Navier-Stokes Equations!

Mechanics:

- Weds 11/5: 3B Symposium!
- PS7 material last on Test 2... Due next Weds.
- Today: mid-term course evaluations!

Muddy from last time:

- In fluids, is τ a shear or normal stress? Equating it to σ is confusing... It's a shear stress. It might have "normal" components, but if you rotate it right, it's all shear.
- What's the difference between a liquid and a Newtonian fluid? Liquids are fluids, as are gases, and plasmas. Definition: finite (nonzero) shear strain rate for small stresses. Bingham plastic not technically a fluid, nor in a sense is a strict power-law pseudoplastic (though tends to break down near 0).

The Navier-Stokes equations! Pinnacle of complexity and abstraction in this course. From here, we explain, we see more examples, we fill in more details. Probably last time without a motivating process... So don't be surprised if you don't understand all of this just now, it's a bunch of math but should be clearer as we go on.

3.21 "Are you ready for momentum convection?"

Conservation of mass 2-D Navier-Stokes: two equations for three unknowns! Need one more equation, conservation of mass, only in-out by convective mass flux $\rho\vec{u}$, no mass diffusion or generation:

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot(\rho\vec{u})$$

$$\frac{\partial\rho}{\partial t} + \vec{u}\cdot\nabla\rho + \rho\nabla\cdot\vec{u} = 0$$

$$\frac{D\rho}{Dt} + \rho\nabla\cdot\vec{u} = 0$$

Incompressible definition: $D\rho/Dt = 0$. Example: oil and water, discuss $D\rho/Dt$ and $\partial\rho/\partial t$. Incompressible, not constant/uniform density. Result: $\nabla\cdot\vec{u} = 0$.

Eulerian derivation of Navier-Stokes Like before; this time add convective momentum transfer. What's that? In convective mass transfer it was $\rho c_p\vec{u}T$. Now it's $\rho\vec{u}\vec{u}$. Wierd outer product second-rank tensor!

But what is momentum convection? Those $u_y\frac{\partial u_x}{\partial y}$ terms. We'll come back to those later. Recall heat transfer with convection:

$$\rho c_p\frac{\partial T}{\partial t} + \nabla\cdot(\rho c_p\vec{u}T) = -\nabla\cdot\vec{q} + \dot{q}$$

With fluids, it's the same:

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla\cdot(\rho\vec{u}\vec{u}) = -\nabla p - \nabla\cdot\tau + \vec{F}$$

Left side expansion, simplification:

$$\rho\frac{\partial\vec{u}}{\partial t} + \vec{u}\frac{\partial\rho}{\partial t} + \rho\vec{u}\nabla\cdot\vec{u} + \rho\vec{u}\cdot\nabla\vec{u} + \vec{u}\vec{u}\cdot\nabla\rho = \vec{u}\left[\frac{\partial\rho}{\partial t} + \vec{u}\cdot\nabla\rho + \rho\nabla\cdot\vec{u}\right] + \rho\left[\frac{\partial\vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right]$$

Recall the continuity equation:

$$\frac{\partial\rho}{\partial t} + \vec{u}\cdot\nabla\rho + \rho\nabla\cdot\vec{u} = 0.$$

Entire first part cancels! Result:

$$\rho\frac{D\vec{u}}{Dt} = -\nabla p - \nabla\cdot\tau + \vec{F}.$$

Now with Newtonian viscosity, incompressible:

$$\tau = -\mu\left(\nabla\vec{u} + \nabla\vec{u}^T - \frac{2}{3}\nabla\cdot\vec{u}I\right).$$

For x-component in 2-D:

$$\tau_x = -\mu\left[2\frac{\partial u_x}{\partial x}\hat{\imath} + \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\hat{\jmath}\right]$$

$$-\nabla\cdot\tau_x = \mu\left[2\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_y}{\partial x\partial y}\right] = \mu\left[\nabla^2 u_x + \frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right)\right]$$

So, that simplifies things quite a bit.

Incompressible Newtonian result:

$$\rho\frac{Du_x}{Dt} = -\frac{\partial p}{\partial x} + \mu\nabla^2 u_x + F_x$$

Written out in 3-D:

$$\rho\left(\frac{\partial u_x}{\partial t} + u_x\frac{\partial u_x}{\partial x} + u_y\frac{\partial u_x}{\partial y} + u_z\frac{\partial u_x}{\partial z}\right) = -\partial p/\partial x + \mu\left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2}\right) + F_x$$

Identify (nonlinear) convective, viscous shear "friction" terms, sources.

The full thing in vector notation:

$$\rho\frac{D\vec{u}}{Dt} = -\nabla p + \mu\nabla^2\vec{u} + \vec{F}$$

Pretty cool. Again, sorta like the diffusion equation.

[For more on this, including substantial derivative, see 2000 David Dussault material, and "omitted" paragraphs from 2001.]

4.6 November 5, 2003: Using the Navier-Stokes Equations

Mechanics:

- Tonight: 3B Symposium! Dinner 5:30 in Chipman room.
- New PS7 on Stellar: no TODO, #4c graph on W^{3}R p. 188.
- Midterm Course Evals:
  - Lectures mostly positive, cards great (one: takes too long); negatives: 1/3 too fast, 1/2 math-intense; need concept summaries.
  - TA: split, most comfortable, 1/3 unhelpful, many: recs need more PS help. “Makes the class not hurt so badly.”
  - PSes: most like, old PSes a prob, need more probs for test studying.
  - Test: like policy, but too long.
  - Text: few helpful different approach, most useless! But better...
  - Time: from 2-5 or 3+ to 12-18; “4 PS + 2-4 banging head against wall.”

Muddy from last time:

- When we started momentum conservation, we had a P, but at the end, only ρ. Where did the P go? Still there. General equations:

$$\frac{D\rho}{Dt} + \rho\nabla\cdot\vec{u} = 0$$
$$\rho\frac{D\vec{u}}{Dt} = -\nabla P - \nabla\cdot\tau + \vec{F}$$

  Incompressible, Newtonian, uniform μ:

$$\nabla\cdot\vec{u} = 0$$
$$\rho\frac{D\vec{u}}{Dt} = -\nabla P + \mu\nabla^2\vec{u} + \vec{F}$$

- Fifth equation in compressible flows: $\rho(P)$, e.g. ideal gas $\rho = MP/RT$.

Convective momentum transfer That nonlinear $D\vec{u}/Dt$ part that makes these equations such a pain!
Example: $t = 0 \to u_x = 1$, $u_y = 2x$, sketch, show at $t = 0$ and $t = 1$. Convecting eddies in background velocity.

Using the Navier-Stokes Equations Handout, start with full equations and cancel terms. Flow through tube revisited. Longitudinal pressure trick with z-derivative of z-momentum equation:

$$\frac{\partial^2 P}{\partial z^2} = \frac{\partial}{\partial z}\left[\frac{\mu}{r}\frac{\partial}{\partial r}\left(\frac{\partial u_z}{\partial r}\right)\right] = \frac{\mu}{r}\frac{\partial}{\partial r}\left(\frac{\partial^2 u_z}{\partial r\partial z}\right) = 0!\ P = A(r,\theta)z + B(r,\theta)$$

$$0 = -\frac{\partial P}{\partial z} + \frac{\mu}{r}\frac{\partial}{\partial r}\left(\frac{\partial u_z}{\partial r}\right) \Rightarrow u_z = \frac{\partial P/\partial z}{4\mu}r^2 + A\ln r + B = -\frac{P_1 - P_2}{4\mu L}z^2 + A\ln r + B.$$

Lateral pressure: if $\theta = 0$ points up:

$$\rho g_r = -\rho g\cos\theta = \partial P/\partial r,$$
$$\rho g_\theta = \rho g\sin\theta = (1/r)\partial P/\partial\theta.$$

Resulting pressure:

$$P = -\rho g r\cos\theta + f(z) = f(z) - \rho g h,$$

for h increasing in the upward direction from z-axis. Final result:

$$P = Az - \rho g h + C.$$

4.7 November 7, 2003: Drag Force

Mechanics:

- New PS7 on Stellar: no TODO, #4c graph on W^3R p. 188.
- Midterm Course Evals:
  - Lectures mostly positive, cards great (one: takes too long); negatives: 1/3 too fast, 1/2 math-intense; need concept summaries.
  - TA: split, most comfortable, 1/3 unhelpful, many: recs need more PS help. "Makes the class not hurt so badly."
  - PSes: most like, old PSes a prob, need more probs for test studying. Bad: last material in last lecture before due! This time: option Weds/Fri, okay?
  - Test: like policy, but too long, too long delay to retake.
  - Text: few helpful different approach, most useless! But better...
  - Time: from 2-5 or 3+ to 12-18; "4 PS + 2-4 banging head against wall."
- Test 2 in less than two weeks... Shorter wait for retake this time.

Muddy from last time:

- Redo pressure derivation.

  $$\frac{\partial^2 P}{\partial z^2} = \frac{\partial}{\partial z}\left[\frac{\mu}{r}\frac{\partial}{\partial r}\left(\frac{\partial u_z}{\partial r}\right)\right] = \frac{\mu}{r}\frac{\partial}{\partial r}\left(\frac{\partial^2 u_z}{\partial r \partial z}\right) = 0!\ P = A(r,\theta)z + B(r,\theta)$$

  Lateral pressure: if $\theta = 0$ points up:

  $$\rho g_r = -\rho g \cos\theta = \partial P/\partial r,$$

  $$\rho g_\theta = \rho g \sin\theta = (1/r)\partial P/\partial\theta.$$

  Resulting pressure:

  $$P = -\rho g r \cos\theta + f(z) = f(z) - \rho g h,$$

  for h increasing in the upward direction from z-axis. Final result:

  $$P = Az - \rho g h + C.$$

- What's fully-developed, edge effects in cylindrical coordinates? Flow direction derivatives deal with fully-developed. If axisymmetric and flow is mostly θ, then can use this as "fully-developed".

  Edge effects: flow direction, large variation direction, third direction is "edge" direction. For tube flow, was θ, so axisymm is equiv to "no edge effects". For rod-cup, will be something else.

Drag force Integrated traction (force per unit area) in one direction. For tubes, it's in the z-direction, use the shear traction (stress) times area: $F_d = \tau \cdot A$. Here, looking at τ_{rz}:

$$u_z = \frac{P_1 - P_2}{4\mu L}(R^2 - r^2) \Rightarrow \tau_{rz} = -\mu\frac{\partial u_z}{\partial r} = \frac{P_1 - P_2}{2L}r.$$

$$F_d = 2\pi RL \cdot \tau_{rz}|_{r=R} = 2\pi RL\frac{P_1 - P_2}{2L}R = \pi R^2(P_1 - P_2).$$

Neat result: this is just the net pressure force. Okay, what if we know desired velocity, want to estimate required pressure? In terms of u_{av}:

$$u_{av} = \frac{u_{max}}{2} = \frac{(P_1 - P_2)R^2}{8\mu L},$$

$$F_d = \frac{(P_1 - P_2)R^2}{8\mu L} \cdot 8\pi\mu L = 8\pi\mu L u_{av}.$$

For any laminar flow, this is the drag force. Drag is shear traction times area:

$$F_d = \tau_{rz} \cdot 2\pi R L \Rightarrow \tau_{rz} = \frac{F_d}{2\pi R L} = \frac{8\pi\mu L u_{av}}{2\pi R L} = \frac{4\mu}{R} u_{av} = \frac{8\mu}{d} u_{av}.$$

Okay, using u_{av} to correlate with flow rate whether laminar or turbulent. So what about turbulent? Density plays a role because of convective terms. Dimensional analysis:

$$\tau = f(U, \mu, d, \rho)$$

Five parameters, three base units, so two dimensionless parameters. Four different nondimensionalizations!

Keep	π_τ	π_{other}
τ, μ	$\frac{\tau}{\rho U^2}$	$\pi_\mu = \frac{\mu}{\rho U d}$
τ, ρ	$\frac{\tau d}{\mu U}$	$\pi_\rho = \frac{\rho U d}{\mu}$
τ, U	$\frac{\tau d^2 \rho}{\mu^2}$	$\pi_U = \frac{\rho U d}{\mu}$
τ, d	$\frac{\tau}{\rho U^2}$	$\pi_d = \frac{\rho U d}{\mu}$

First and last are essentially the same, though last is more familiar (Reynolds number), so ignore the first. Third is just a mess, so throw it out. Second is a great fit to what's above. So use last, or second?

With turbulence, there are different curves with different surface roughnesses, roughly proportional to U^2. If use second, get one flat π_τ laminar, multiple lines for turbulent π_τ. If use first/last, one line for laminar, multiple flats for turbulance (p. 188). So this is generally more convenient.

Dimensionless π_τ is called (fanning) friction factor f (f_f). The denominator $\frac{1}{2}\rho U^2$ is the approximate kinetic energy density, we'll call it K, a.k.a. dynamic pressure. So:

$$\tau = fK, \; F_d = fKA, f = \frac{\tau}{\frac{1}{2}\rho U^2} = f(\mathrm{Re}).$$

Laminar flow friction factor:

$$f = \frac{\tau}{\frac{1}{2}\rho U^2} = \frac{\frac{8\mu}{d} u_{av}}{\frac{1}{2}\rho U^2} = \frac{16\mu}{\rho U d} = \frac{16}{\mathrm{Re}}.$$

To calculate drag force: Reynolds number (and surface roughness) → friction factor $f \rightarrow \tau = fK$, $F_d = fKA$.

4.8 November 12, 2003: Drag Force on a Sphere

Mechanics:

- Test 2 11/19 in 2-143, preview handout today.
- PS7 extended to Friday.

Muddy from last time:

- How is $f = 16\mu/\rho U d$?

$$\tau_{rz} = \frac{8\mu}{d} u_{av} \Rightarrow f = \frac{\tau_{rz}}{\frac{1}{2}\rho u_{av}^2} = \frac{8\mu u_{av}/d}{\frac{1}{2}\rho u_{av}^2} = \frac{16\mu}{\rho u_{av} d} = \frac{16}{\text{Re}}.$$

- What's the point of defining f? We just need τ, right? Well, f is easy for laminar flow, for turbulence it's more complicated. This gives us a parameter to relate to the Reynolds number for calculating drag force in more general situations. More examples on the way.
- Or was it $\vec{t}$, not f? In that case, traction $\vec{t} = \sigma \cdot \hat{n}$, force per unit area. In this case, with $n = \hat{r}$, $\vec{t} = (\tau_{rr} + p, \tau_{r\theta}, \tau_{rz})$. The relevant one for the z-direction is τ_{rz}, but traction is more general, see an example later today.
- Why was option #4 the "better" graph? Expanded version: with roughness at high Re, f is constant. So if Re=10^8, friction factor is *only* a function of e/d down to $e/d = 10^{-5}$!
- Please review this process $Q \to u_{av} \to \text{Re} \to f \to \tau \to F_d \to \Delta P$.

$$\frac{Q}{\pi R^2} = u_{av},\ \text{Re} = \frac{\rho u_{av} d}{\mu},\ f = f(\text{Re}, e/d),\ \tau_{rz} = fK,\ F_{d,z} = \tau_{rz} A = fKA (A = 2\pi R L),\ \Delta P = \frac{F_d}{\pi R^2}.$$

Reynolds Number revisited Low velocity: shear stress; high velocity: braking kinetic energy. Ratio of forces:

$$\text{Re} = \frac{\text{convective momentum transfer}}{\text{shear momentum transfer}} = \frac{\text{inertial forces}}{\text{viscous forces}} \simeq \frac{\rho u_y \frac{\partial u_x}{\partial y}}{\mu \frac{\partial^2 u_x}{\partial y^2}} \simeq \frac{\rho U U/L}{\mu U/L^2} = \frac{\rho U L}{\mu}.$$

Flow past a sphere Motivating process: Electron beam melting and refining of titanium alloys. Water-cooled copper hearth, titanium melted by electron beams, forms solid "skull" against the copper. Clean heat source, liquid titanium contained in solid titanium, results in very clean metal. Mystery of the universe: how does liquid Ti sit in contact with solid Cu? Main purpose: removal of hard TiN inclusions often several milimeters across which nucleate cracks and bring down airplanes! (1983 Sioux City, Iowa.)

Set up problem: sphere going one way u_{sphere}, fluid other way u_∞, local disturbance but relative velocity $U = u_\infty - u_{sphere}$, relative veloc of fluid in sphere frame. Drag force is in this direction.

For a sphere, drag force is slightly different: it has not only shear, but pressure component as well. Traction $\vec{t} = \sigma \cdot \hat{n}$. Stokes flow: ingore the convective terms, result (pp. 68-71):

$$F_d = 3\pi \mu d u_{rel}.$$

At high velocity, similar friction factor concept to tube:

$$F_d = fKA = f \cdot \frac{1}{2}\rho U^2 \cdot \frac{1}{4}\pi d^2.$$

Again, $f(\text{Re})$, but not really π_τ because τ is all over the place, more of an average. This time, low Re (<0.1) means Stokes flow, can ignore all convective terms; analytical result in 3.21 notes, drag force:

$$F_d = 3\pi\mu U d = f \cdot \frac{1}{2}\rho U^2 \cdot \frac{1}{4}\pi d^2 \Rightarrow f = \frac{24\mu}{\rho U d} = \frac{24}{\text{Re}}.$$

If faster, though not turbulent, f becomes a constant. Graph on W^{3}R p. 153 of f (they call c_D) vs. Re. Constant: about 0.44, that's what I've known as the drag coefficient. Cars as low as 0.17, flat disk just about 1, making dynamic pressure a good estimate of pressure difference.

For rising/sinking particles, set drag force to buoyancy force, solve for velocity. If not Stokes flow, you're in trouble, way to do it but it's complicated.

Can *NOT* use this for bubbles. For those, $F_d = 2\pi\mu U d$ all the way out to Re=10^5!

So, what about precipitation? Buoyancy force and weight vs. drag force, all sum to zero:

$$F_w = \frac{1}{6}\pi d^3 \rho_{sphere}, F_b = \frac{1}{6}\pi d^3 \rho_{fluid}, F_d = \text{what we just calculated.}$$

After all, if you're not part of the solution, you're part of the precipitate. (Ha ha)

4.9 November 14, 2003: Boundary Layers Part I

Mechanics:

- Wulff Lecture Tues 4:15 6-120: *Information Transport and Computation in Nanometer-Scale Structures*, Don Eigler, IBM Fellow.
- Test 2 11/19 in 2-143. Solving Fluids Problems provided if needed.
- PS7 solution error: #1 replace L with δ, "length" with L. Correction on Stellar.

Muddy from last time:

- Which are the convective and viscous terms? In vector Navier-Stokes momentum:

  $$\rho \frac{D\vec{u}}{Dt} = \rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right) = -\nabla P + \mu\nabla^2\vec{u} + \vec{F}.$$

  Convective terms are the $\vec{u}\cdot\nabla\vec{u}$ terms, like $u_x \partial u_y/\partial x$, the nonlinear terms which make the equations such a pain to solve and create turbulence... Viscous ones are $\mu\nabla^2\vec{u}$.
- Why do thin ellipsoids have less drag than spheres, but flat plates have more? Depends on orientation. P&G has a few more examples on p. 87. Neat thing: the Stokes flow $f = 24/\mathrm{Re}$ holds for all of them!
- Are $\log(f)$ vs. $\log(\mathrm{Re})$ plots for only turbulent, or both laminar and turbulent? Both, that's the neat thing. For tube, sphere, and BL, it captures everything.

Sphere flow wrapup Another neat way to think about Re: ratio of inertial to shear forces

$$\frac{\rho U^2 \cdot \pi d^2}{\mu d U} \propto \frac{\rho U d}{\mu} = \mathrm{Re}.$$

Can *NOT* use this flow-past-sphere stuff for bubbles. For those, $F_d = 2\pi\mu U d$ all the way out to Re$=10^5$! Boundary conditions...

"Boundary layers" in a solid Thought experiment with moving solid: extruded polymer sheet (like PS4 extruded rod problem). Start at high temp, if well-cooled so large Biot then constant temperature on surface; no generation. Full equation:

$$\frac{DT}{Dt} = \alpha\nabla^2 T$$

Define boundary layer thickness δx where temperature deviates at least 1% from far-field. If $\delta \ll x$, then

$$\frac{\partial^2 T}{\partial y^2} >> \frac{\partial^2 T}{\partial x^2}$$

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

Transform: $\tau = x/u_x$, becomes diffusion equation, erf solution:

$$\frac{T - T_s}{T_i - T_s} = \mathrm{erf}\frac{y}{2\sqrt{\alpha x/u_x}}$$

If we define δ as where we get to 0.99, then $\mathrm{erf}^{-1}(.99) = 1.8$, and

$$y = \delta \text{ where } \frac{\delta}{2\sqrt{\alpha x/u_x}} = 1.8$$

$$\delta = 3.6\sqrt{\frac{\alpha x}{u_x}}$$

Obviously breaks down at start $x = 0$, but otherwise sound.

Boundary layers in a fluid Now we want to calculate drag force for flow parallel to the plate.

Similar constant IC to solid, infinite BC, call it U_∞. Difference: BC at $y = 0$: $u_x = u_y = 0$. Have to solve 2-D incompressible steady-state Navier-Stokes:

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0$$

$$u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} = -\frac{\partial p}{\rho \partial x} + \nu \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial x^2} \right)$$

$$u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} = -\frac{\partial p}{\rho \partial y} + \nu \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial x^2} \right)$$

Then a miracle occurs, the Blassius solution for $\delta \ll x$ is a graph of u_x/U_∞ vs. $\beta = y\sqrt{U_\infty/\nu x}$; hits 0.99 at ordinate of 5:

$$\delta = 5.0\sqrt{\frac{\nu x}{U_\infty}}.$$

Why 5.0, not 3.6? Because there must be vertical velocity due to mass conservation (show using differential mass equation and integral box), carries low-x-velocity fluid upward. Slope: 0.332, will use next time to discuss shear stress and drag force.

4.10 November 17, 2003: Boundary Layers Part II

Mechanics:

- Wulff Lecture Tues 4:15 6-120: *Information Transport and Computation in Nanometer-Scale Structures*, Don Eigler, IBM Fellow.
- PS7 solution error: #1 replace L with δ, "length" with L. Correction on Stellar.
- Zephyr hours tomorrow 9-12, 1-3; also Weds 4-7 PM.
- Test 2 11/19 in 2-143. Solving Fluids Problems provided if needed.

Muddy from last time:

- Nothing!

Recall our "miraculous" Blassius solution to the 2-D Navier-Stokes equations (draw the graph)... At $y = 0$, slope: 0.332, so viscous drag:

$$\tau_{yx} = -\mu \frac{\partial u_x}{\partial y} = -\mu \frac{\partial u_x}{\partial \beta} \frac{\partial \beta}{\partial y}$$

$$\tau_{yx} = -\mu \cdot 0.332 U_\infty \sqrt{\frac{U_\infty}{\nu x}}$$

Note: a function of x (larger near leading edge), diverges at $x = 0$! But $\delta \ll x$ does not hold there.

Now set to a friction factor:

$$\tau_{yx} = -0.332 \sqrt{\frac{\rho \mu U_\infty^3}{x}} = f_x \cdot \frac{1}{2} \rho U_\infty^2$$

This time τ is not constant, so we have different $f_x = \tau / K$ and $f_L = F_d / KA$. Let's evaluate both:

$$f_x = 0.664 \sqrt{\frac{\mu}{\rho U_\infty x}} = \frac{0.664}{\sqrt{\mathrm{Re}_x}}$$

Also, note dimensionless BL thickness:

$$\delta = 5.0 \sqrt{\frac{\nu x}{U_\infty}}$$

$$\frac{\delta}{x} = 5.0 \sqrt{\frac{\nu}{U_\infty x}} = \frac{5.0}{\sqrt{\mathrm{Re}_x}}$$

Lengthwise, global drag force, average friction factor. Neglect edge effects again...

$$F_d = \int \tau_{yx} dA = W \int_{x=0}^{L} tau_{yx} dx$$

$$F_d = W \int_{x=0}^{L} 0.332 \sqrt{\frac{\rho \mu U_\infty^3}{x}} dx$$

$$F_d = 0.332 W \sqrt{\rho \mu U_\infty^3} \cdot 2 \sqrt{L}$$

$$F_d = 0.664 W \sqrt{\rho \mu U_\infty^3 L}$$

Now for the average friction factor/drag coefficient:

$$f_L = \frac{F_d}{KA} = \frac{0.664 W \sqrt{\rho \mu U_\infty^3 L}}{\frac{1}{2} \rho U_\infty^2 \cdot WL} = 1.328 \sqrt{\frac{\mu}{\rho U_\infty L}} = \frac{1.328}{\sqrt{\mathrm{Re}_L}}$$

This is what is meant by average and local friction factors on the Test 2 overview sheet. Don't need to know for test 2, since for a tube they're the same. For a sphere, only defined average/global, but for a BL, they're different.

Entrance Length For channel flow between two parallel plates spaced apart a distance H, we can define the entrance length L_e as the point where the boundary layers from each side meet in the middle. The twin Blassius functions are close enough to the parabolic profile that we can say it's fully-developed at that point. So we can plug in the boundary layer equation if flow is laminar:

$$x = L_e \Rightarrow \frac{H}{2} = \delta = 5.0\sqrt{\frac{\nu x}{U_\infty}},$$

$$L_e = \frac{H^2 U_\infty}{100\nu}.$$

If $L_e \ll L$, then flow is fully-developed for most of the tube, so the fully-developed part will dominate the drag force and $F_d = \tau \cdot 2\pi R L$.

Movie Friday...

4.11 November 21, 2003: Turbulence

Mechanics:

- Turbulence movie: QC151.T8; guide QC145.2.F5 Barker Media.

Muddy from last time:

- What's the physical significance of "Blassius"? Some guy who came up with this function to solve a slightly-reduced 2-D Navier-Stokes. There are actually three, for u_x, u_y and p in the boundary layer, all $\delta \ll x$. For drag force, only u_x is needed.
- Is $dBL/d\beta$ only the slope at the initial part of the curve? If by "initial", you mean $y = 0$ (the bottom), then yes.
- What's the difference between f_x and f_L? Here, τ is not constant, graph τ and $\tau_{av} \rightarrow F_d$, show how average is twice local at the end. Hence f_L is twice f_x.
- How about "Re_x" and "Re_L"? No significance, just different lengthscales, one for local and one for global/average.
- Difference between u_{av} and U_∞? Should be no u_{av} for BL problems, sorry if I made a writo. D'oh! This is wrong, see next lecture's notes.
- What's up with δ/x? Just a ratio, dimensionless for convenience, allows to evaluate $\delta \ll x$.
- What is velocity profile for entrance length if not laminar? Get to that later (next Monday or so).
- What happens near leading edge? Something like the sphere: kinda complicated. Maybe solvable for Stokes flow...

Turbulence Starting instability, energy cascade. Vortices grow in a velocity gradient because of momentum convection, damped due to viscosity; therefore, tendency increases with increasing Re.

Resulting behavior:

- Disorder.
- "Vorticity" in flow, 3-D.
- Lots of mixing, of mass and heat as well as momentum.
- Increased drag due to momentum mixing, as small vortices steal energy from the flow.

The movie!

Parviz Moin and John Kim, "Tackling Turbulence with Supercomputers," *Scientific American* January 1997 pp. 62-68.

> Turbulence may have gotten its bad reputation because dealing with it mathematically is one of the most notoriously thorny problems of classical physics. For a phenomenon that is literally ubiquitous, remarkably little of a quantitative nature is known about it. Richard Feynman, the great Nobel Prize-winning physicist, called turbulence "the most important problem of classical physics." Its difficulty was wittily expressed in 1932 by the British physicist Horace Lamb, who, in an address to the British Association for the Advancement of Science, reportedly said, "I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic."

That article goes on to talk about direct numerical simulation of all of the details of turbulent flows, of which I am not a great fan. Why? as pointed out in my *JOM* article “3-D or not 3-D”, even if computers continue to double in computational power every eighteen months, the fifth-power scaling of complexity with lengthscale in three dimensions (cubic in space times quadratic in time) means that the resolution of these simulations will double only every seven-and-a-half years!

To take a simple illustrative example, direct numerical simulation of turbulence in continuous casting involves Reynolds numbers on the order of one million, and the smallest eddies are a fraction of a millimeter across and form and decay in a few milliseconds. One must account for interaction with the free surface, including mold powder melting and entrainment, as well as mold oscillation, and surface roughness of the solidifying metal, since with turbulent flow, the details of these boundary conditions can make a large difference in macroscopic behavior. The formulation alone is daunting, and computational work required to solve all of the equations on each of the tens of trillions of grid points over the millions of timesteps required to approach steady-state will be prohibitively costly for many years, perhaps until long after Moore’s law has been laid to rest (indeed, the roughly four petabytes of memory required to just store a single timestep would cost about two billion dollars at the time this is being written). Furthermore, postprocessing that many degrees of freedom would not only be computationally difficult, but it is not clear that our minds would be able to comprehend the resulting complexity in any useful way, and further, the exercise would be largely pointless, as one really cares only about coarse-grained averages of flow behavior, and detailed behavior perhaps at certain interfaces.

Analysis: for 1 $\frac{\mathrm{m}}{\mathrm{s}}$ flow through the nozzle 0.1 m in diameter, with kinematic viscosity of $.005/7000 \simeq 10^{-6}$ $\frac{\mathrm{m}^2}{\mathrm{s}}$, this gives us $\mathrm{Re}_d \simeq 10^5$. Using the larger lengthscale H of the caster, around 1 m, this gives $\mathrm{Re}_H \simeq 10^6$, this is given in the paragraph above. Using standard enengy cascade/Kolmogorov microscale analysis, the energy dissipation rate for the largest turbulent eddies in a tube is given by

$$\epsilon \sim \mu_t \left(\frac{U}{d}\right)^2,$$

where μ_t is the turbulent viscosity, U the eddy velocity estimated by the average velocity, and d the eddy size estimated by the tube diameter. Combining this with the well-known Kolmogorov result for the smallest eddy lengthscale ℓ:

$$\ell \sim \sqrt[4]{\frac{\mu^3}{\rho^2 \epsilon}}$$

(ρ is density) gives the smallest eddy lengthscale as

$$\ell \sim d \frac{1}{\sqrt{\mathrm{Re}_d}} \sqrt[4]{\frac{\mu}{\mu_t}}.$$

Even using the conservative estimate of $\mu_t = 30\mu$ gives $\ell \sim 0.1$ mm, in 1 meter cubed this gives a trillion grid points, but you want a few grid points across each smallest eddy which means about a $\text{few}^3 \simeq 100$ times more grid points, hence “tens of trillions”.

Put slightly differently, the total rate of energy dissipated in a jet at steady-state is the rate of kinetic energy input, which is the product of volumetric kinetic energy given by dynamic pressure and the flow rate:

$$\epsilon V = \frac{1}{2}\rho U^2 \cdot \frac{\pi}{4} d^2 U = \frac{\pi}{8}\rho U^3 d^2$$

Taking the volume as 1 m^3, average velocity of 1 $\frac{\mathrm{m}}{\mathrm{s}}$, nozzle diameter of 0.1 m and density of 7000 $\frac{\mathrm{kg}}{\mathrm{m}^3}$ gives $\epsilon \simeq 30 \frac{\mathrm{W}}{\mathrm{m}^3}$. Putting this into the Kolmogorov lengthscale expression again gives $\ell \sim 0.1$ mm.

4.12 November 24, 2003: Turbulence, cont'd

Mechanics:

- Turbulence movie: QC151.T8; guide QC145.2.F5 Barker Media.

Muddy from last time:

- Difference between u_{av} and U_∞? I messed up last time, for the entrance length situaiton, we we take average velocity as U_∞, the initial "free stream" velocity. Sorry to confuse you last time.
- On that note, just as we have the dimensionless boundary layer thickness, we also have the dimensionless entrance length:
$$L_e = \frac{H^2 u_{av}}{100\nu} \Rightarrow \frac{L_e}{H} = \frac{\mathrm{Re}_H}{100}.$$
So a large Reynolds number means a long entrance length (1000 means ten times the channel width), and vice versa.

Energy cascade and the Kolmogorov microscale. Largest eddy Re=UL/ν, smallest eddy Reynolds number $u\ell/\nu \sim 1$. Energy dissipation, W/m^3; in smallest eddies:

$$\epsilon = \eta \left(\frac{du}{dx}\right)^2 \sim \eta \frac{u^2}{\ell^2}$$

Assuming most energy dissipation happens there, we can solve these two equations, get smallest eddy size and velocity from viscosity, density and dissipation:

$$u \sim \ell \sqrt{\frac{\epsilon}{\eta}} \Rightarrow \frac{\rho \ell^2}{\eta}\sqrt{\frac{\epsilon}{\eta}} \sim 1$$

$$\ell \sim \left(\frac{\eta^3}{\rho^2 \epsilon}\right)^{\frac{1}{4}}$$

This defines the turbulent microscale. For thermal or diffusive mixing, turbulence can mix things down to this scale, then molecular diffusion or heat conduction has to do the rest. Time to diffusive mixing in turbulence is approximately this ℓ^2/D.

So suppose we turn off the power, then what happens? Smallest eddies go away fast, then larger ones, until the whole flow stops. Timescale of smallest is ℓ^2/ν, largest is L^2/ν_t, turbulent effective viscosity. Get into modeling and structure later if time is available.

Turbulent boundary layer Laminar is good until $\mathrm{Re}_x = 10^5$, associated boundary layer thickness and local friction factor:

$$\frac{\delta}{x} = \frac{5.0}{\sqrt{\mathrm{Re}_x}},\ f_x = \frac{0.664}{\sqrt{\mathrm{Re}_x}},\ f_L = \frac{1.328}{\sqrt{\mathrm{Re}_L}},$$

In range 10^5 to 10^7, transition, oscillatory; beyond 10^7 fully turbulent. Always retains a laminar sublayer against the wall, though it oscillates as vortices spiral down into it. New behavior:

$$\frac{\delta}{x} = \frac{0.37}{\mathrm{Re}_x^{0.2}}$$

So $\delta \sim x^{0.8}$. Grows much faster. Why? Mixing of momentum, higher effective velocity. But still a laminar sublayer near the side.

f_x is oscillating all over the place, but what about the new f_L? Disagreement, even for smooth plate:

$$\text{P\&G p. 38}: f_L = \frac{0.455}{(\log \mathrm{Re}_L)^{2.58}};\ \text{BSL p. 203}: f_L = \frac{0.146}{\mathrm{Re}_L^{0.2}}$$

Either way get some kind of curve in f-Re space which jumps in turbulence. W^{3}R doesn't give an f_L, just an f_x on p. 179, which is:

$$f_x = \frac{0.0576}{(\mathrm{Re}_x)^{0.2}}.$$

Time-smoothing Time smoothing, or experiment-smoothing and Reynolds stresses: velocity varies wildly, decompose into $u_x = \bar{u}_x + u'_x$, where $\bar{u}$ is time-smoothed:

$$\bar{u}_x = \frac{\int_{t_a}^{t_b} u_x dt}{t_b - t_a}.$$

For time-dependent, experiment-average it.

Contest Prizes Wednesday for those who catch the two errors in the Navier-Stokes equations t-shirt!

Not covered this year The following topics were not covered in lecture, but are here for your edification if you're interested.

Reynolds stresses Then take time-smoothed transport equations:

$$\frac{\partial(\bar{u}_x \bar{+} u'_x)}{\partial t} = \frac{\partial\bar{\bar{u}}_x}{\partial t} + \frac{\partial\bar{u'_x}}{\partial t} = \frac{\partial\bar{u}_x}{\partial t} + 0.$$

Same with spatial derivatives, pressure terms. But one thing which doesn't time-smooth out:

$$u'_x \frac{\partial u'_x}{\partial x} \neq 0.$$

This forms the Reynolds stresses, which we shift to the right side of the equation:

$$\tau_{xy} = -\mu \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) - \rho \bar{u'_x u'_y}$$

Show how it's zero in the center of channel flow, large near the sides, zero *at* the sides. The resulting mass equation is the same; x-momentum equation:

$$\rho \left(\frac{\partial \bar{u}}{\partial t} + \bar{\vec{u}} \cdot \nabla \bar{u}_x \right) = -\frac{\partial \bar{P}}{\partial x} + \mu \nabla^2 \bar{u}_x - \rho \left(\frac{\partial}{\partial x}(\rho u'_x u'_x) + \frac{\partial}{\partial y}(\rho u'_x u'_y) + \frac{\partial}{\partial z}(\rho u'_x u'_z) \right) + F_x.$$

Turbulent transport and modeling Recall on test: pseudoplastic, Bingham. Define effective viscosity: shear stress/strain rate.

On a micro scale, lots of vortices/eddies. On a macro scale, mixing leads to higher effective D_t, k_t, and η_t at length scales down to that smallest eddy size, less so close to walls. All three turbulent diffusivities have the same magnitude.

New dimensionless number: Prandtl number is ratio of ν to diffusivity, e.g. ν/D and ν/α. $\mathrm{Pr}_t \simeq 1$ for heat and mass transfer.

Next time: thermal and solutal boundary layers, heat and mass transfer coefficients, turbulent boundary layer, then natural convection. Last, Bernoulli equation, continuous reactors.

Modeling: $K - \ell$ and $K - \epsilon$ modeling (C_μ, C_1, C_2, σ_K and σ_ϵ are empirical constants):

$$K = \frac{1}{2}\rho(u'^2_x + u'^2_y + u'^2_z), \nu_t = C_\mu \frac{K^2}{\epsilon}.$$

$$\frac{DK}{Dt} = \nabla \cdot \left(\frac{\nu_t}{\sigma_K} \nabla K \right) + \nu_t \nabla\vec{u} \cdot \left(\nabla\vec{u} + (\nabla\vec{u})^T \right) - \epsilon.$$

$$\frac{D\epsilon}{Dt} = \nabla \cdot \left(\frac{\nu_t}{\sigma_\epsilon} \nabla \epsilon \right) + C_1 \frac{\nu_t \epsilon}{K} \nabla\vec{u} \cdot (\nabla\vec{u} + (\nabla\vec{u})^T) - C_2 \frac{\epsilon^2}{K}.$$

Chapter 5

Coupled Fluids with Heat and Mass Transfer

5.1 November 26, 2003: Coupled Fluids, Heat and Mass Transfer!

Mechanics:

- Congrats to Jenny and David for winning the contest, prize: $5 Tosci's.
- PS8 on Stellar, due Fri 12/5.
- Evaluations next Wednesday 12/3.

Muddy from last time:

- Time smoothing: what are u_x, $\bar{u}_x$, u'_x? They are: the real velocity, the time-smoothed component of velocity, and the fluctuating component of velocity.
- What timescale can you find from the lengthscale of the smallest eddies? How would one go about this? Two timescales are relevant here: one is diffusion timescale ℓ^2/D, which gives mixing time, and the timescale of formation and elimination of these little eddies ℓ^2/ν. When attempting direct numerical simulation of turbulence, this tells how small a timestep one will need (actually, a fraction of this for accuracy); this also describes how long the eddies will last after the mixing power is turned off.

Thermal and solutal boundary layers Types: forced, natural convection; forced today, natural later.

Recall first BL thought experiment on thick polymer sheet extrusion, hot polymer sheet T_∞ and cold water T_s. Now it's happening in a liquid, competing thermal and fluid boundary layers with thicknesses δ_u and δ_T.

Fluid:

$$\delta_u = 5.0\sqrt{\frac{\nu x}{U_\infty}}$$

Thermal if flow uniform, same criterion:

$$\delta_T = 3.6\sqrt{\frac{\alpha x}{U_\infty}}$$

Dimensionless:

$$\frac{\delta_T}{x} = \frac{3.6}{\sqrt{\frac{U_\infty x}{\alpha}}} = \frac{3.6}{\sqrt{\mathrm{Re}_x \mathrm{Pr}}}$$

When is flow uniform? In a solid, or for much larger thermal boundary layer than fluid, so $\alpha >> \nu$, Pr$<< 1$.

Another way to look at it:

$$\frac{\delta_T}{\delta_u} = 0.72\text{Pr}^{-1/2}$$

Large Prandtl number (>.5) means

$$\frac{\delta_T}{\delta_u} = 0.975\text{Pr}^{-1/3}$$

Liquid metals (and about nothing else) have small Pr; mass transfer Pr is almost always large. *E.g.* water $\nu = 10^{-6}\frac{\text{m}^2}{\text{s}} = 10^{-2}\frac{\text{cm}^2}{\text{s}}$, but D is typically around $10^{-5}\frac{\text{cm}^2}{\text{s}}$.

Note: blood platelets diffuse at around $D = 10^{-9}$, but tumbling blood cells not only stir and increase diffusivity, but somehow platelets end up on the sides of blood vessels, where they're needed. I don't fully understand...

Heat and Mass Transfer Coefficients What about h? Start with h_x, then h_L, as before with f_x and f_L. Let $\beta_T = y\sqrt{U_\infty/\alpha x}$, $\theta = T - T_s/T_\infty - T_s$, graph θ vs. β_T gives $\theta = \text{erf}(\beta_T/2)$.

Heat conduction into the liquid:

$$q_y = -k\frac{\partial T}{\partial y} = -k\frac{dT}{d\theta}\frac{d\theta}{d\beta_T}\frac{\partial \beta_T}{\partial y}$$

$$q_y = k(T_s - T_\infty)\frac{1}{\sqrt{\pi}}\sqrt{\frac{U_\infty}{\alpha x}} = h_x(T_s - T_\infty)$$

$$h_x = \frac{k}{\sqrt{\pi}}\sqrt{\frac{U_\infty}{\alpha x}} = \sqrt{\frac{k\rho c_p U_\infty}{\pi x}}$$

Likewise for mass transfer, ρc_p is effectively one, so:

$$h_{Dx} = \sqrt{\frac{DU_\infty}{\pi x}}$$

Next time: average, dimensional analysis, $\delta_T < \delta_u$ case.

5.2 December 1, 2003: Nusselt Number, Heat and Mass Transfer Coefficients

Mechanics:

- Evals Wednesday.

Muddy from last time:

- In the thermal boundary layer with constant velocity, why is $\partial^2 T/\partial x^2 << \partial^2 T/\partial y^2$? That's because $\delta \ll x$, so graph T vs. x and vs. y, show y-deriv is larger.
- Is there a physical meaning behind $\delta_T/\delta_u \propto \mathrm{Pr}^{-1/2}$ and $\delta_C/\delta_u \propto \mathrm{Pr}^{-1/3}$? Yes, see below.

Heat and mass transfer coefficients Recap last time:

- Flow and heat/mass transfer: weakly coupled. So far, all laminar.
- Case 1: much larger thermal(/concentration) boundary layer (Pr<0.1): consider T/C BL to have uniform velocity, use same BL formulation as moving solid motivating example: erf solution, $\delta_T = 3.6\sqrt{\alpha x/U_\infty}$. Here:
$$\delta_C/\delta_u \text{ or } \delta_T/\delta_u = 0.72\mathrm{Pr}^{-1/2}.$$
Physical meaning: grows as sqrt of diffusivity, so ratio is ratio of square roots of diffusivity, which is inverse sqrt(Pr).
- Case 2: smaller thermal(/concentration) boundary layer (Pr>5 or so): consider T/C BL to have linear velocity, smaller velocity means thicker T/C BL. Here:
$$\delta_C/\delta_u \text{ or } \delta_T/\delta_u = 0.975\mathrm{Pr}^{-1/3}.$$
- Moving on, back to case 1, calculated $q|_{y=0}$ from erf solution:
$$q_y = k(T_s - T_\infty)\frac{1}{\sqrt{\pi}}\sqrt{\frac{U_\infty}{\alpha x}} = h_x(T_s - T_\infty) \Rightarrow h_x = \sqrt{\frac{k\rho c_p U_\infty}{\pi x}}.$$
Likewise for mass transfer:
$$h_{Dx} = \sqrt{\frac{DU_\infty}{\pi x}}.$$

Since that's the local, let's integrate for average, neglecting edge effects:

$$q_{av} = \frac{1}{WL}\int_{x=0}^{L} h_x(T_s - T_\infty)W\,dx = h_L(T_s - T_\infty)$$
$$\frac{2(T_s - T_\infty)}{L}\left[\sqrt{k\rho c_p U_\infty x/\pi}\right]_{x=0}^{L} = h_L(T_s - T_\infty)$$
$$h_L = 2\sqrt{\frac{k\rho c_p U_\infty}{\pi L}} = 2h_x|_{x=L}$$

Now for case 2 (high-Prandtl), need different formulation. Dimensional analysis of mass transfer:

$$h_D = f(D_{fl}, U, x, \nu)$$

Five parameters, two base units (cm, s), so three dimensionless. Eliminate x and D. Then one dimensionless is Reynolds (π_U), one is Prandtl (π_ν), what's the third?

$$\pi_{h_D} = \frac{h_D x}{D_{fl}}$$

Looks like the Biot number, right? But it's not, it's actually quite different.

$$\mathrm{Bi} = \frac{h_D L}{D_{solid}} = \frac{L/D_{solid}}{1/h} = \frac{\text{Resistance to conduction in solid}}{\text{Resistance due to BL in liquid}}$$

Uses L=solid thickness, D_{solid}. Heat transfer note: you get one extra dimensionless number, due to heating by viscous friction.

Here, Nusselt #, L=length of plate (in flow direction), the conduction and BL are in the same medium, use D_{liquid}.

$$\mathrm{Nu} = \frac{h_D L}{D_{liquid}} = \frac{L}{D_{liquid}/h_D} \simeq \frac{L}{\delta_C} \text{ or } \frac{L}{\delta_T}.$$

Low-Prandtl fit:

$$\frac{h_L L}{k} = 2\sqrt{\frac{U_\infty L}{\pi \alpha}} = \frac{2}{\sqrt{\pi}} \mathrm{Re}_L^{1/2} \mathrm{Pr}^{1/2}$$

Actually, for small to "medium" Pr, slight correction:

$$\mathrm{Nu}_x = \frac{0.564 \mathrm{Re}_x^{1/2} \mathrm{Pr}^{1/2}}{1 + 0.90\sqrt{\mathrm{Pr}}}$$

$$\mathrm{Nu}_L = \frac{1.128 \mathrm{Re}_x^{1/2} \mathrm{Pr}^{1/2}}{1 + 0.90\sqrt{\mathrm{Pr}}}$$

High: (>0.6): nice derivation in $\mathrm{W}^3\mathrm{R}$ chapter 19:

$$\mathrm{Nu}_x = 0.332 \mathrm{Re}_x^{1/2} \mathrm{Pr}^{0.343}$$

$$\mathrm{Nu}_L = 0.664 \mathrm{Re}_L^{1/2} \mathrm{Pr}^{0.343}$$

Just as there are more correlations for f (friction factor), lots more correlations for various geometries etc. in handout by 2001 TA Adam Nolte. Summarize: flow gives Re, props give Pr, gives Nu, gives h (maybe Bi).

5.3 December 3: Natural Convection

Mechanics:

- Course evals today!

Muddy from last time:

- What's the relationship between h_x or h_L and the friction factor? Hmm... Meaning: heat transfer coefficient, kinetic energy transfer coefficient. Types: local, global/average. Laminar flow variation: both$\sim 1/\sqrt{x}$, integral$\sim \sqrt{x}$, average$\sim 1/\sqrt{x}$. Laminar $f_L = 2f_x|_{x=L}$, $h_L = 2h_x|_{x=L}$. Dimensionless: $f = f(\text{Re})$, Nu=f(Re,Pr). Different correlations for different geometries.
- Other Nusselt numbers from sheet by Adam Nolte. (Note for Re=0 with a sphere...)

Natural convection Hot stuff rises, cold stuff sinks. Obvious examples: radiators, etc. Strongly-coupled equations:

$$\frac{D\rho}{Dt} + \nabla \cdot \vec{u} = 0$$

$$\rho \frac{D\vec{u}}{Dt} = -\nabla p + \eta \nabla^2 \vec{u} + \rho \vec{g}$$

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

Full coupling comes in the ρ in the fluid flow equations.

Volumetric thermal expansion coefficient:

$$\beta = -\frac{1}{\rho}\frac{d\rho}{dT},\ \rho - \rho_0 = \beta(T - T_0)$$

Note relation to 3.11 thermal expansion coeff:

$$\alpha = \frac{1}{L}\frac{dL}{dT}$$

$$\beta = -\frac{1}{\rho}\frac{d\rho}{dT} = -\frac{V}{M}\frac{d(M/V)}{dT}$$

$$d(1/V) = -dV/V^2,\ dV = d(L^3) = 3L^2 dL$$

$$\beta = V\frac{dV}{V^2 dT} = \frac{3L^2 dL}{V dT} = \frac{3}{L}\frac{dL}{dT} = 3\alpha.$$

Word explanation: heat a solid cube, length increases 1% in each direction, volume increases 3%. Both have units $1/K$. Ideal gases:

$$\rho = \frac{P}{RT},\ \beta = -\frac{1}{\rho}\frac{d\rho}{dT} = -\frac{RT}{P}\left(-\frac{P}{RT^2}\right) = 1/T.$$

Also $\beta_C = -\frac{1}{\rho}\frac{d\rho}{dC}$.

Simplest case: vertical wall, T_s at wall, T_∞ with density ρ_∞ away from it, x vertical and y horizontal for consistency with forced convection BL. Assume:

1. Uniform kinematic viscosity $\nu = \nu_\infty$.
2. Small density differences: ρ only matters in ρg term, otherwise ρ_∞ for convective terms.
3. Steady-state.
4. Boussinesq approx: $p \simeq -\rho_\infty g x + \mathit{const}$, obvious away from BL, no pressure difference across BL to drive flow.

5. Also with small density diff: $\Delta\rho/\rho = \beta\Delta T$ (ρ is roughly linear with T).
6. No edge effects (z-direction).

With assumptions 1 and 2, get momentum equation:

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = \nu_\infty \nabla^2 \vec{u} + \frac{1}{\rho_\infty} \left(\rho \vec{g} - \nabla p \right).$$

Now for x-momentum, steady-state (assumption 3), assumption 4 gives:

$$\vec{u} \cdot \nabla u_x = \nu_\infty \nabla^2 u_x + \frac{-\rho g + \rho_\infty g}{\rho_\infty}$$

Now assumptions 5 and 6, x-momentum becomes:

$$u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} = \nu_\infty \nabla^2 u_x + g\beta(T - T_\infty)$$

With $T_s > T_\infty$ and $g_x = -g$, this gives driving force in the positive-x direction, which is up, like it's supposed to. Okay, that's all for today, more next time.

5.4 December 5: Wrapup Natural Convection

Mechanics:

- Test 2: before max=90, mean 75.38, std. dev 12.23; after max=100, mean 95.76, std. dev 6.37.

Muddy from last time:

- D'oh! Left too early...

Last time: assumptions led to equation:

$$u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} = \nu_\infty \nabla^2 u_x + g\beta(T - T_\infty)$$

One more assumption, $\delta_u \ll x$, gives:

$$u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} = \nu_\infty \frac{\partial^2 u_x}{\partial y^2} + g\beta(T - T_\infty)$$

New dimensional analysis:

$$h = f(x, \nu, k, \rho c_p, g\beta, T_s - T_\infty)$$

Seven params 4 base units (kg, m, s, K); 3 dimless params. Again Pr (dim'less ρc_p), Nu (dim'less h), this time Grashof number (dim'less β).

$$\mathrm{Gr} = \frac{g\beta(T_s - T_\infty)L^3}{\nu^2}$$

Forced convection: $\mathrm{Nu} = f(\mathrm{Re}, \mathrm{Pr})$.
Natural convection: $\mathrm{Nu} = f(\mathrm{Gr}, \mathrm{Pr})$.
Detour: recall falling film

$$u_x = \frac{g \sin\theta (2Lz - z^2)}{2\nu}$$

$$u_a v = \frac{g \sin\theta L^2}{3\nu}$$

$$\mathrm{Re} = \frac{u_a v \delta}{\nu} = \frac{g \cos\beta \delta^3}{3\nu^2}$$

So Gr is a natural convection Reynolds number, determines the rate of growth of the BL.

Graphs of dimensionless $T = (T - T_\infty)/(T_s - T_\infty)$, dimensionless $u_x = \mathrm{Re}_x / 2\sqrt{\mathrm{Gr}_x}$ vs. $y/\sqrt[4]{Gr_x}$ on P&G p. 232 corresponding to dimensional graphs in W^{3}R p. 313. Explain velocity BL is always at least as thick as thermal BL, but thermal can be thinner for large Pr.

Forced convection: $\delta \propto \sqrt{x}$
Natural convection: $\delta \propto \sqrt[4]{x}$
Note: in P&G p. 232 plots, Pr=0.72 corresponds to air.
Another Gr interpretation: dimensionless temperature gradient; for $\theta = \frac{T - T_\infty}{T_s - T_\infty}$:

$$\frac{\partial T}{\partial y} = \frac{\partial T}{\partial \theta} \frac{\partial \theta}{\partial \frac{y}{x} \sqrt[4]{\frac{Gr_x}{4}}} \frac{1}{x} \sqrt[4]{\frac{Gr_x}{4}} = (T_s - T_\infty) f(\mathrm{Pr}) \frac{1}{x} \sqrt[4]{\frac{Gr_x}{4}}$$

Note velocity squared proportional to driving force in pipe flow, kinda same here; heat trans proportional to square root of velocity. Hence $\mathrm{Re}_x \propto \sqrt{\mathrm{Gr}_x}$ for velocity, $\mathrm{Nu_x} \propto \sqrt{\mathrm{Re_x}} \propto \sqrt[4]{\mathrm{Gr}_x}$.

Transition to turbulence determined by Ra=GrPr, boundary at 10^9. Laminar, Ra between 10^4 and 10^9:

$$\frac{\mathrm{Nu}_L}{\sqrt[4]{\mathrm{Gr}_L/4}} = \frac{0.902 \mathrm{Pr}^{1/2}}{(0.861 + \mathrm{Pr})^{1/4}}$$

Special for $0.6 < \mathrm{Pr} < 10$, laminar:

$$\mathrm{Nu}_L = 0.56(\mathrm{Gr}_L\mathrm{Pr})^{1/4}$$

Turbulence, Ra between 10^9 and 10^{12} (p. 259):

$$\mathrm{Nu}_L = \frac{0.0246\mathrm{Gr}_L^{2/5}Pr^{7/15}}{(1+0.494\mathrm{Pr}^{2/3})^{2/5}}$$

Again, velocity$^{0.8}$ in a way, sorta like turbulent forced convection boundary layers.

5.5 December 8: Wrapup Natural Convection, Streamfunction and Vorticity

Mechanics:

- Final exam Monday 12/15 in 4-149. Discuss operation, incl. closed/open sections, new diff eq, essay.

Muddy from last time:

- What were we supposed to get out of the last lecture? Pretty much the list given: how natural conv BLs work, calculate $h_{(D)L}$ using Nu_L, $\delta_u \geq \delta_T$ or δ_C, natural BLs grow more slowly, velocity and temperature profiles.
- What direction is velocity? Dominant velocity is in x-direction, which is vertical; upward for hot wall, downward for cold. What's the difference between velocity in the BL, far from it? Far from it, velocity is zero.
- Why $\delta_u \geq \delta_T$? Hot region lifts (or cold region sinks) fluid, so all of the hot/cold region (thermal BL) will be moving (in the velocity BL). For large Pr, $\nu > \alpha$, so the momentum diffusion happens faster, thin thermal and thick velocity.
- Dimensionless curves: crazy non-intuitive axis value $\frac{y}{x}\sqrt[4]{\mathrm{Gr}_x/4}$! Well, not much worse than Blassius: u_x/U_∞ vs. $\beta = y\sqrt{U_\infty/\nu x} = \frac{y}{x}\sqrt{\mathrm{Re}_x}$. But I'll give you that the dimensionless velocity is a bit odd.
- Where do these things come from? Okay. Concretize:

$$\frac{\frac{u_x x}{\nu}}{2\sqrt{\mathrm{Gr}_x}} = \frac{1}{2}\frac{u_x x}{\nu}\sqrt{\frac{\nu^2}{g\beta\Delta T x^3}} = \frac{u_x}{\sqrt{g\beta\Delta T x}} \Rightarrow u_{x,max} = f(\mathrm{Pr})\sqrt{g\beta\Delta T x}.$$

$$\frac{\delta_u}{x}\sqrt[4]{\frac{\mathrm{Gr}_x}{4}} = f(\mathrm{Pr}) \Rightarrow \delta_u = f(\mathrm{Pr})\frac{x}{\sqrt[4]{\mathrm{Gr}_x/4}} = \sqrt{2}f(\mathrm{Pr})\sqrt[4]{\frac{x^4\nu^2}{g\beta\Delta T x^3}} = \sqrt{2}f(\mathrm{Pr})\sqrt[4]{\frac{x\nu^2}{g\beta\Delta T}}.$$

These two results are consistent with: $u_{x,max} \propto \text{thickness}^2$, forced convection $\Delta u_x/\Delta y$ goes as $1/\sqrt{\mathrm{Re}_x}$.

Other geometries: Raylegh-Bernard cells in inversion for GrPr greater than 1000. Solutal buoyancy too, dissolving salt cube.

$$\beta_C = -\frac{1}{\rho}\frac{d\rho}{dC}.$$

Special: nucleate boiling, film boiling, h vs. T with liquid coolant.

If time: BL on rotating disk: $u \propto r$, so uniform BL. Pretty cool.

Now can calculate (estimate) heat/mass transfer coefficients for forced and natural convection, laminar or turbulent. (D'oh! Forgot this closing part after the muddy stuff.)

Stream Function and Vorticity Vorticity introduced in turbulence video, measure of local rotation, definition:

$$\omega = \nabla \times \vec{u}$$

2-D scalar, 3-D vector. Some formulations give 2-D NS in terms of u_x, u_y, ω. Also, vorticity particle methods: bundles of vorticity moving, combining, annihilating.

Other application: crystal rotation in semisolid rheology.

Stream function, for incompressible flow where $\nabla \cdot \vec{u} = 0$:

$$u_x = \frac{\partial \Psi}{\partial y},\ u_y = -\frac{\partial \Psi}{\partial x}$$

Collapses velocity components into one parameter. Look at $\Psi = Ax$, $\Psi = By$, $\Psi = Ax + By$, $\Psi^2 = x^2 + y^2$. Cool.

Gradient is normal to flow direction. Streamlines: curves of constant Ψ, parallel to flow direction. If spaced apart same difference in Ψ, then

$$|\vec{u}| \propto \text{distance between streamlines}$$

Aero-astros look out at wing and see streamline, Mech Es see structure, Mat Scis see a giant fatigue specimen...

Visualizing 2-D flows, giving approximate regions of large and small velocity. DON'T CROSS THE STREAMS!

Concept: flow separation, difference between jet and inlet. Breathing through nose. (D'oh! Forgot to mention breathing through the nose.)

Decisions... Finish the term with the Bernoulli equation, or continuous flow reactors? Bernoulli wins the vote.

5.6 December 10, 2003: Bernoulli, Semester Wrapup

TODO: get rooms for review sessions!

Mechanics:

- Review sessions: me Friday 2 PM, Albert Sunday evening.

No muddy cards from last time.

Bernoulli Equation W^{3}R chap 6: control volume integral derivation based on first law of thermodynamics. Interesting, I do somewhat different, based on Navier-Stokes; I like to think mine is more straightforward, but you can read W^{3}R if needed.

Also called "inviscid flow". Motivation: tub with hole, pretty close to zero friction factor, velocity is infinity? No. Something other than viscosity limits it.

Navier-Stokes, throw out viscous terms:

$$\rho\frac{D\vec{u}}{Dt} = -\nabla p + \rho\vec{g}$$

Change coordinates to local streamline frame: $\hat{s}$ in direction of flow, $\hat{n}$ in direction of curvature (perpendicular in 2-D, complicated in 3-D).

Flow only in s-direction, s-momentum equation for $\vec{g} = -g\hat{z}$:

$$\rho\left(\frac{\partial u_s}{\partial t} + u_s\frac{\partial u_s}{\partial s}\right) = -\frac{\partial p}{\partial s} + \rho g_z\frac{\partial z}{\partial s}$$

Steady-state, constant ρ:

$$\frac{\partial\left(\frac{1}{2}\rho u_s^2\right)}{\partial s} + \frac{\partial p}{\partial s} - \rho g_z\frac{dz}{ds} = 0$$

Integrate along a streamline:

$$\frac{1}{2}\rho V^2 + p + \rho g z = constant$$

In other words:

$$KE + P + PE = constant$$

This is the Bernoulli equation.

Example 1: draining tub with a hole in the bottom. Set $z = 0$ at the bottom: PE=ρgh at top, P at bottom corner is that plus atmospheric pressure, $\frac{1}{2}\rho V^2$ beyond outlet (further accelerating). Potential energy becomes pressure $\Delta P = \rho gh$, then becomes kinetic $V = \sqrt{2gh}$.

Illustrate how changes with long tube h_2 down from bottom: ρgh at top, P_0 at base in corner, $\frac{1}{2}\rho V^2 + P_1$ at base over spout, $\frac{1}{2}\rho V^2 - \rho g h_2$ at tube end. Three equations in three unknowns. Solves to $P_1 = \rho gh$, $V^2 = 2g(h + h_2)$, $P_1 = -\rho g h_2$. Can also fill in the table...

Conditions:

- No shear or other losses (not nearly fully-developed)
- No interaction with internal solids, etc.
- No heat in or out, mechanical work on fluid (pumps, etc.)
- No sudden expansion (jet⟶turbulent dissipation, separation complicates stuff)
- No turbulence
- No combustion (mixing⟶effective viscosity)
- *Yes* sudden contraction.

Note time-to-drain problem on final of three years ago (that was the "derive and solve a new equation" problem of 2000), tendency for diff eqs and thought problems...

Semester summary You've come a very long way! Mentioned linear to multiple nonlinear PDEs, understanding of solution. More generally, learned to start with a simple conservation relation: accum = in - out + gen, turn into really powerful results, on macro or micro scale, for diffusion, thermal energy, mass, momentum, even kinetic energy.

Covered all topics in fluid dynamics and heat and mass transfer, in MechE, ChemE, aero-astro. If want to go on, take graduate advanced fluid dynamics or heat/mass transfer, will be bored in undergrad class.

Also done some computation; for more depth with or without programming experience, try 22.00J/3.021J! (Shameless plug...)

Thank Albert for a terrific job as a TA!

Last muddy questions

- What is the relevance of the boundary layer thickness to the Bernoulli equation? The boundary layer is a region where there is quite a bit of shear, and sometimes turbulence. If it is thin relative to the size of the problem (e.g. relative to the diameter of the tube), then most of the fluid will have negligible shear.
- Why such a wierd coordinate system in Bernoulli example 2? Why not just make $z = 0$ at the bottom of the tube? You could do that too, and it would work equally well, it just differs by a constant in the potential energy; the way we did it is just more consistent with the first example:

Point	KE	P	PE
1	∼0	p_{atm}	$\rho g(h_1 + h_2)$
2	∼0	$p_{atm} + \rho g h_1$	$\rho g h_2$
3	$\rho g(h_1 + h_2)$	$p_{atm} - \rho g h_2$	$\rho g h_2$
4	$\rho g(h_1 + h_2)$	p_{atm}	0

Batch and Continuous Flow Reactors For those interested.

Basic definitions, motivating examples. Economics: batch better for flexibility, continuous for quality and no setup time (always on).

Two types: volumetric and surface reactors. Volume V, generation due to chemical reaction; we'll discuss first-order $A \longrightarrow B$, so

$$G = -kC_A$$

For a volume batch reactor, start with $C_{A,in}$, dump into reactor, it goes:

$$\text{accum} = \text{generation}$$

$$V\frac{dC_A}{dt} = -VkC_A$$

$$\ln(C_A) = -kt + A$$

$$\frac{C_{A,out}}{C_{A,in}} = \exp(-kt)$$

For mass transfer-limited surface batch reactor, say

$$\text{accum} = \text{out}$$

$$V\frac{dC_{A,out}}{dt} = -Ah_d C_A$$

$$\frac{C_{A,out}}{C_{A,in}} = \exp\left(-\frac{h_D A}{V}t\right)$$

Two extremes in continuous reactor behavior with flow rate Q: plug flow and perfect mixing.

Plug flow is like a mini-batch with $t_R = V/Q$, draw plug in a pipe, derive:

$$\frac{C_{A,out}}{C_{A,in}} = \exp\left(-\frac{kV}{Q}\right)$$

With a surface, the Vs cancel, left with

$$\frac{C_{A,out}}{C_{A,in}} = \exp\left(-\frac{h_D A}{Q}\right)$$

Perfect mixing: in, out, gen, no accum, out at $C_{A,out}$ reactor conc:

$$0 = QC_{A,in} - QC_{A,out} - kVC_{A,out}$$

$$\frac{C_{A,out}}{C_{A,in}} = \frac{Q}{Q+kV} = \frac{1}{1+\frac{kV}{Q}}$$

With area:

$$\frac{C_{A,out}}{C_{A,in}} = \frac{1}{1+\frac{h_D A}{Q}}$$

Say target conversion is 0.01, given volume V, homogeneous with constant k.

- Batch:

  $$t_R = \frac{1}{k}\ln(C_{A,in}/C_{A,out}) = \frac{4.6}{k}$$

  prodection rate is

  $$\frac{V}{\frac{4.6}{k} + t_{change}} = \frac{kV}{4.6 + kt_{change}}$$

- Plug:

  $$Q = \frac{kV}{\ln(C_{A,in}/C_{A,out})} = \frac{kV}{4.6}$$

  Better than batch, likely better quality too, less flexible.

- Perfect mixing:

  $$Q = \frac{kV}{C_{A,in}/C_{A,out} - 1} = \frac{kV}{99}$$

  Much smaller than either of the others!

Dead zones and effective volumes!

How to tell: tracers, Peclet number.

Other examples: catalytic combustion (that dimensional analysis problem in PS3), alveoli/breathing (continuous/batch mixed). Batch: generally better conversion in same volume (see why); continuous: consistent quality, no setup time.

Steelmaking: batch, but folk want to make continuous.