CBE 30357
BIOLOGICAL TRANSPORT PHENOMENA

8/22/2017

SUMMARY FOR TODAY

- Define "Transport Phenomena" and provide context of this course and the spring course within the curriculum
- Make some observations about chemical engineering in society…
- Describe the overall structure of the course
- Show numerous examples where the subject is relevant

JUNIOR YEAR !!

- This is the year where you get to transition from saying you are a “chemical engineering major” to saying you are a chemical engineer!

Dept. of Chemical and Biomolecular Engineering

Standard Curriculum

	Fall		Spring	
Freshman	MATH 10550, Calculus 1	4	MATH 10560, Calculus 2	4
	CHEM 10171/11171 Intro to Chem	4	CHEM 10122 Gen Chem	3
	EG 10111, Intro to Eng	3	EG 10112, Intro to Eng	3
	Arts & Letters 1	3	PHYS 10310, General Physics 1	4
	University Seminar/A&L 2	3	University Seminar/A&L 3	3
		17		17
Sophomore	MATH 20550, Calculus 3	3.5	MATH 20580, Linear ODEs	3.5
	CHEM 10172/11172, Organic 1 +lab	4	CHEM 20273, Organic 2	3
	CBE 20255, Intro to Chem Eng	3	CBE 20260, Thermodynamics 1	3
	PHYS 10320, Gen Physics 2	4	CBE 20258, Numer. and Stat Methods	3
	A&L 4	3	A&L 5	3
		17.5	*CBE 20290, Career Choices Eng	*1
				15.5 /*16.5
Junior	MATH 30650, Differential Eq	3	CHEM 30324, Pchem	3
	CHEM 30333/31333 Achem & Lab	4	CBE 30338, Chem Proc Control	3
	CBE 30355 Transport 1		CBE 30356, Transport 2	3
	or CBE 30357 Biotransport	3	CBE 31358, Chem Eng Lab 1	3
	CBE 30367, Thermo 2	3	A&L 6	3
	CBE 30361, Materials	3		15
		16		
Senior	CBE 40443, Separations	3	CBE 40448, Process Design	3
	CBE 40445, Reaction Engineering	3	CBE Elective	3
	CBE 41459, Chem Eng Lab 2	3	Tech Elective	3
	CBE Elective	3	Advance Science Elective	3
	A&L 7	3	A&L8	3
		15		15
Total		128 credits	*Strongly recommended	

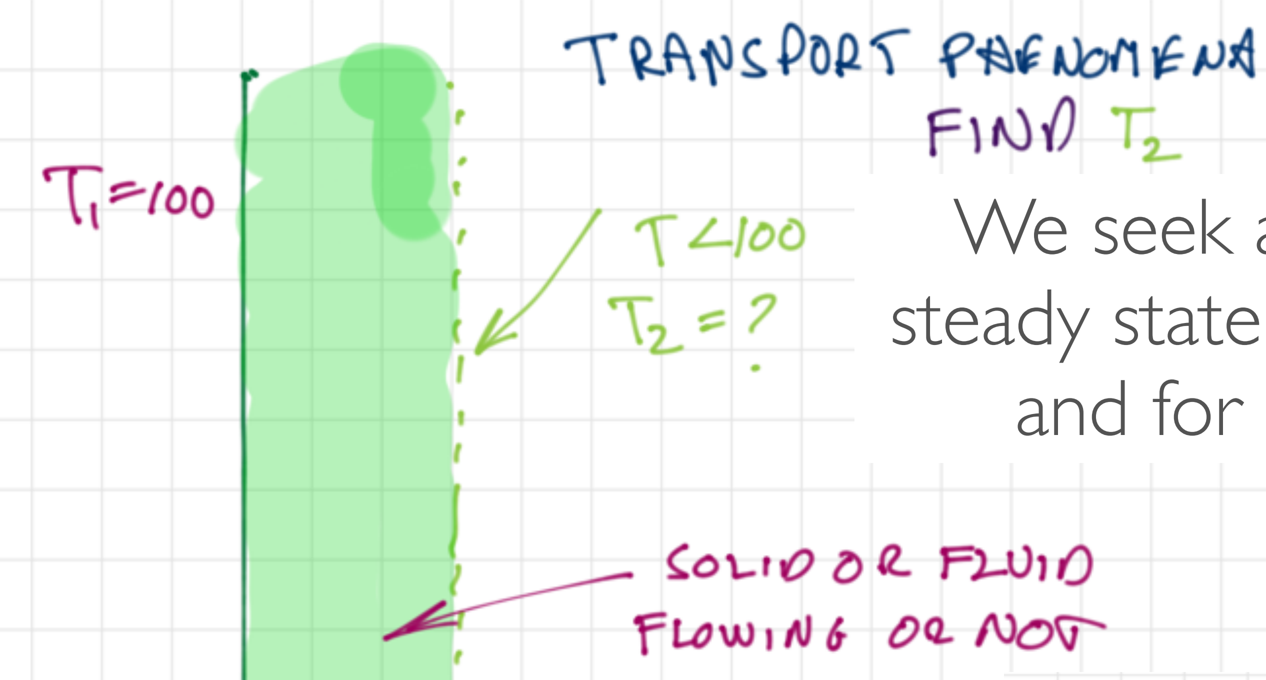
DEGREE OF UNIQUENESS

- **Chemical Thermodynamics**
  - Nobody other than chemical engineers knows anything about this!
- **Transport Phenomena**
  - The mechanical engineers work on some aspects of fluid flow and heat transfer, but generally can't make the connection to the either the molecular scale or the specific chemical/material components of the system
- These are not trivial subjects and even if you did stay at a *Holiday Inn Express* last night, you can't learn them in 3 hours, in a small room on a Saturday morning!

TRANSPORT PHENOMENA

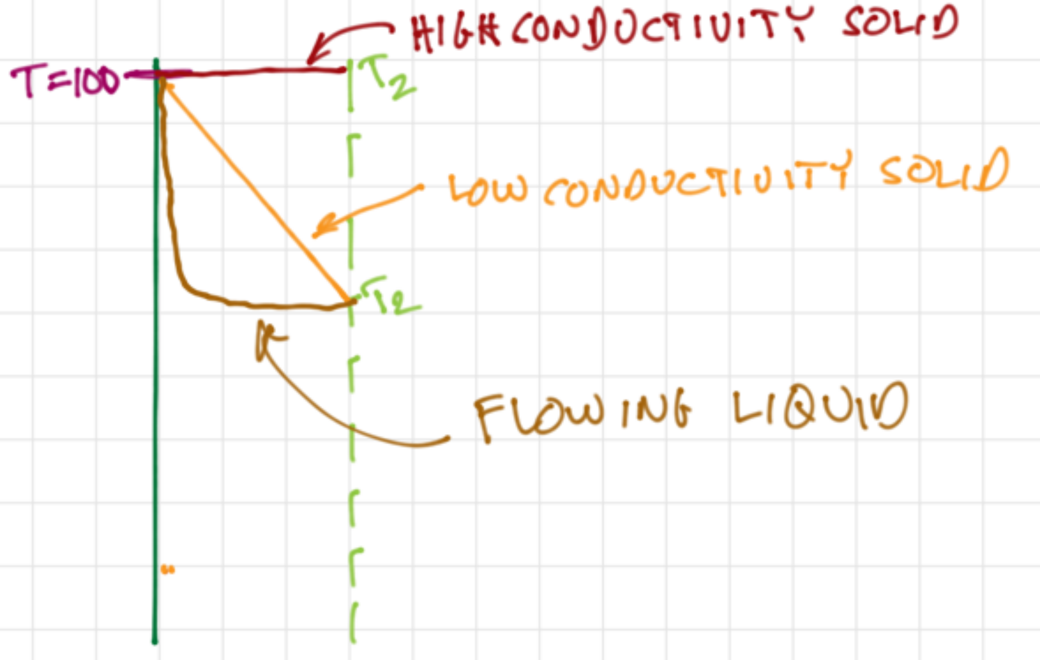
- “Transport phenomena” is the collective term for momentum transport, heat transfer and mass transfer” — collective study is more common in chemical engineering than in mechanical engineering
- Because the basic mechanisms of transport are the same (or similar) for all three quantities,
  - molecular diffusion/conduction
  - convection
- the governing equations are similar and thus study as a coherent subject makes sense. (and is *potentially* optimal.)

BASIC QUESTIONS TO BE ANSWERED



We seek a general answer for steady state or <u>transient</u> situations and for arbitrary materials

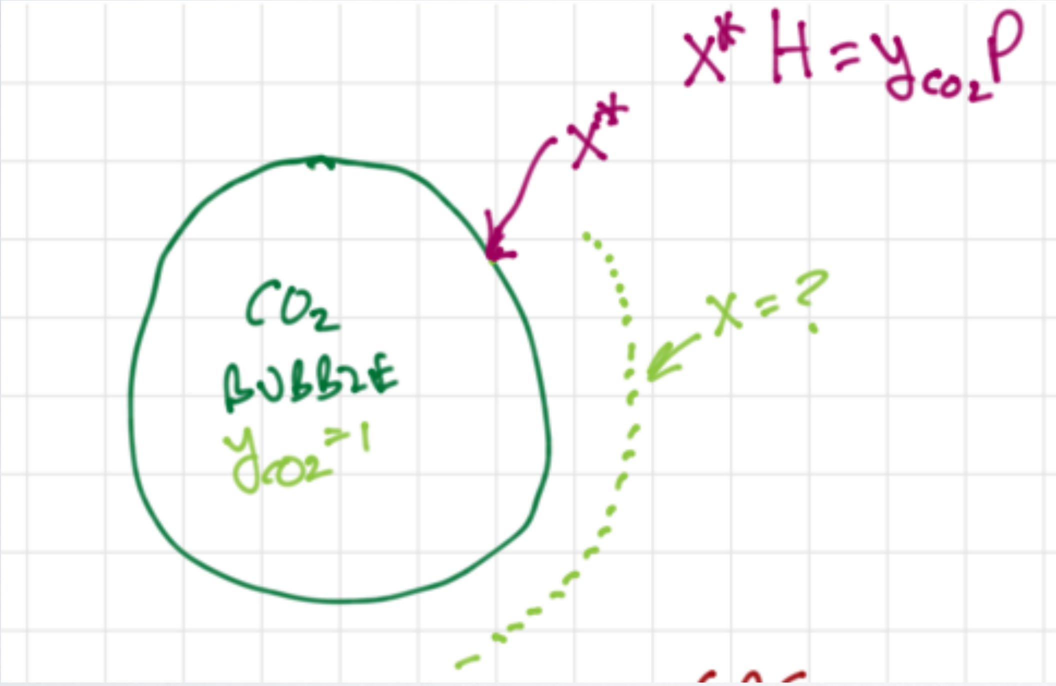
T is fixed at some boundary, we would like the temperature at all distances from the boundary.
We also want the heat "flux".

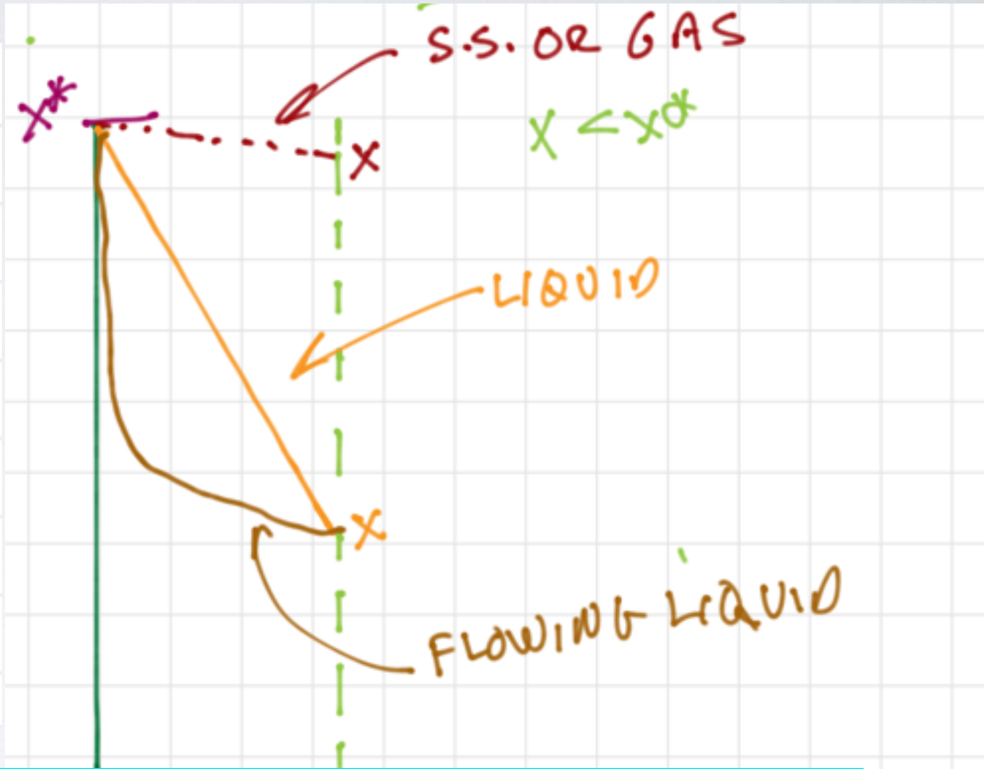


TRANSPORT PHENOMENA

- We want to be able to answer for temperature, concentration or velocity.
- We want to be able to answer for steady state or transient scenarios.
- We need to be able to deal with more complicated "boundary conditions" where a phase change may occur or a chemical reaction is occurring.

MASS TRANSFER

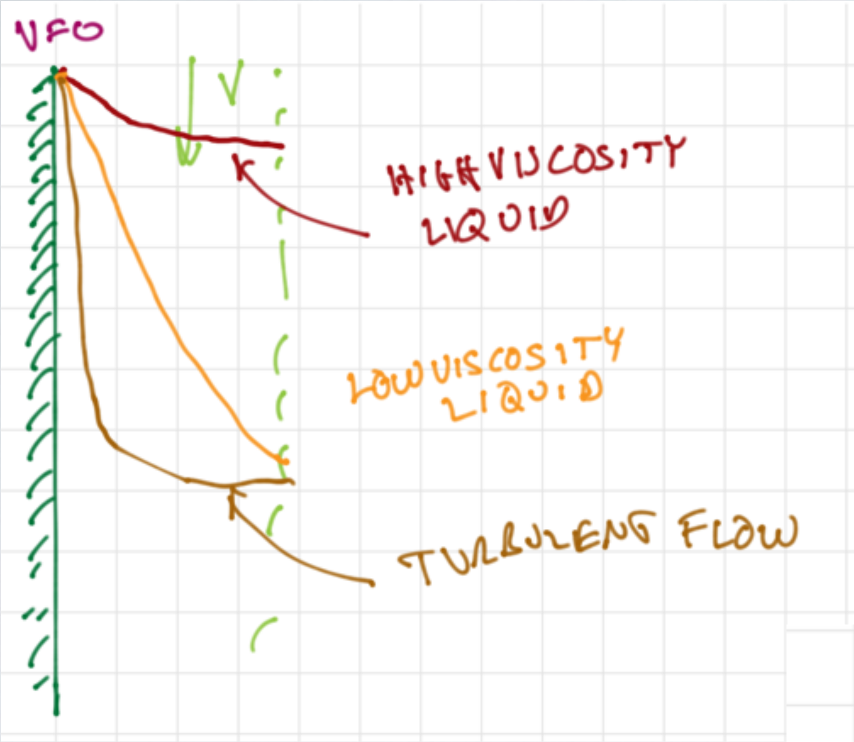




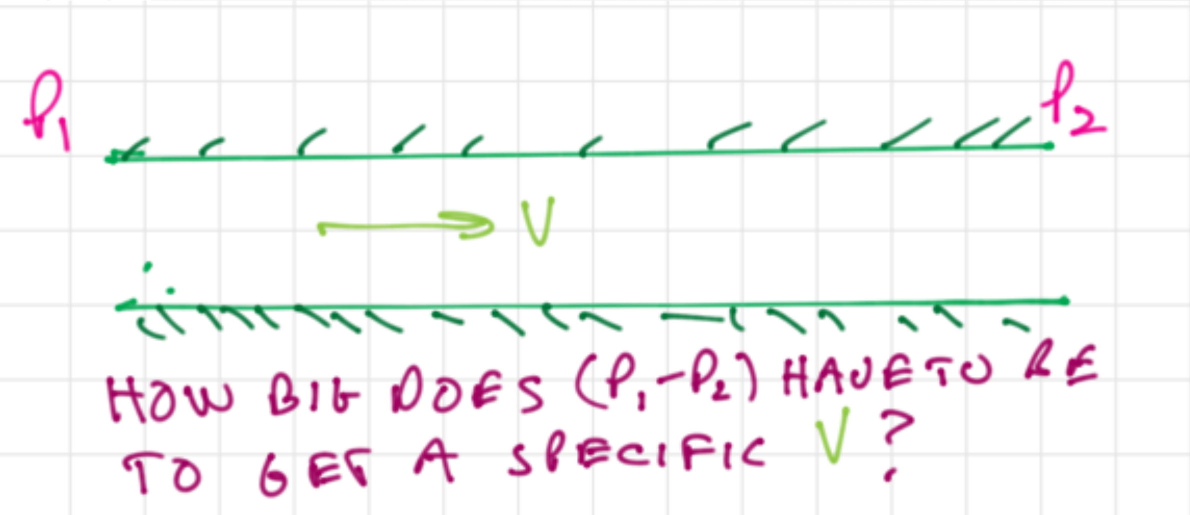
A CO2 bubble is present in a liquid which has a CO2 concentration well below the equilibrium solubility. Thus CO2 will move from the gas bubble into the liquid. How fast will this occur?

What is the concentration of CO2 “near” to the bubble?

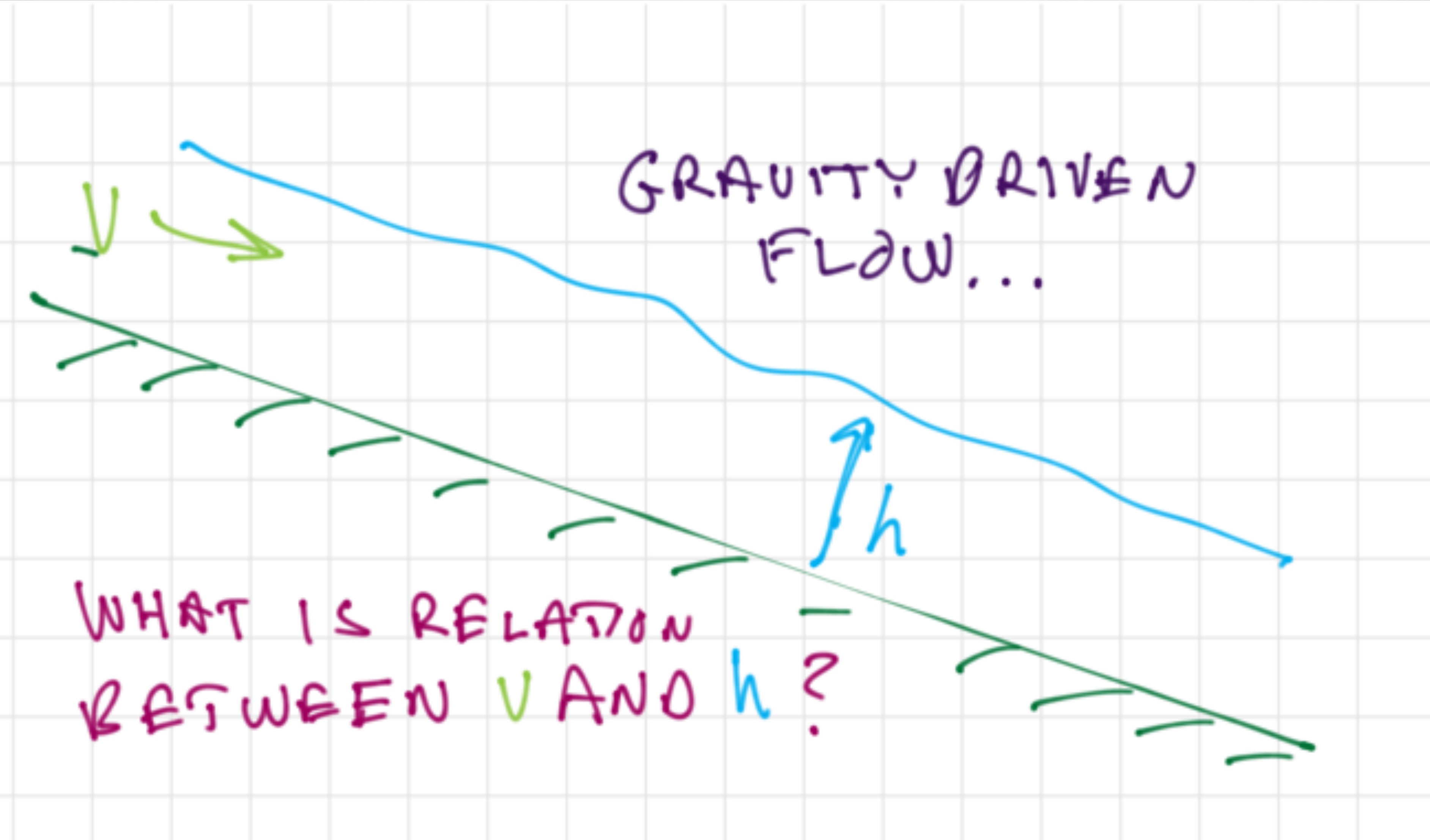
FLUID FLOW CAUSED BY A PRESSURE DIFFERENCE



If the velocity is 0, at the wall, what is the "velocity profile"? What "forcing" is necessary to cause or maintain this flow?



HOW BIG DOES (P_1-P_2) HAVE TO BE TO GET A SPECIFIC V?



WHAT IS RELATION BETWEEN V AND h?

SIMPLEST EQUATION TO DESCRIBE WHAT IS HAPPENING

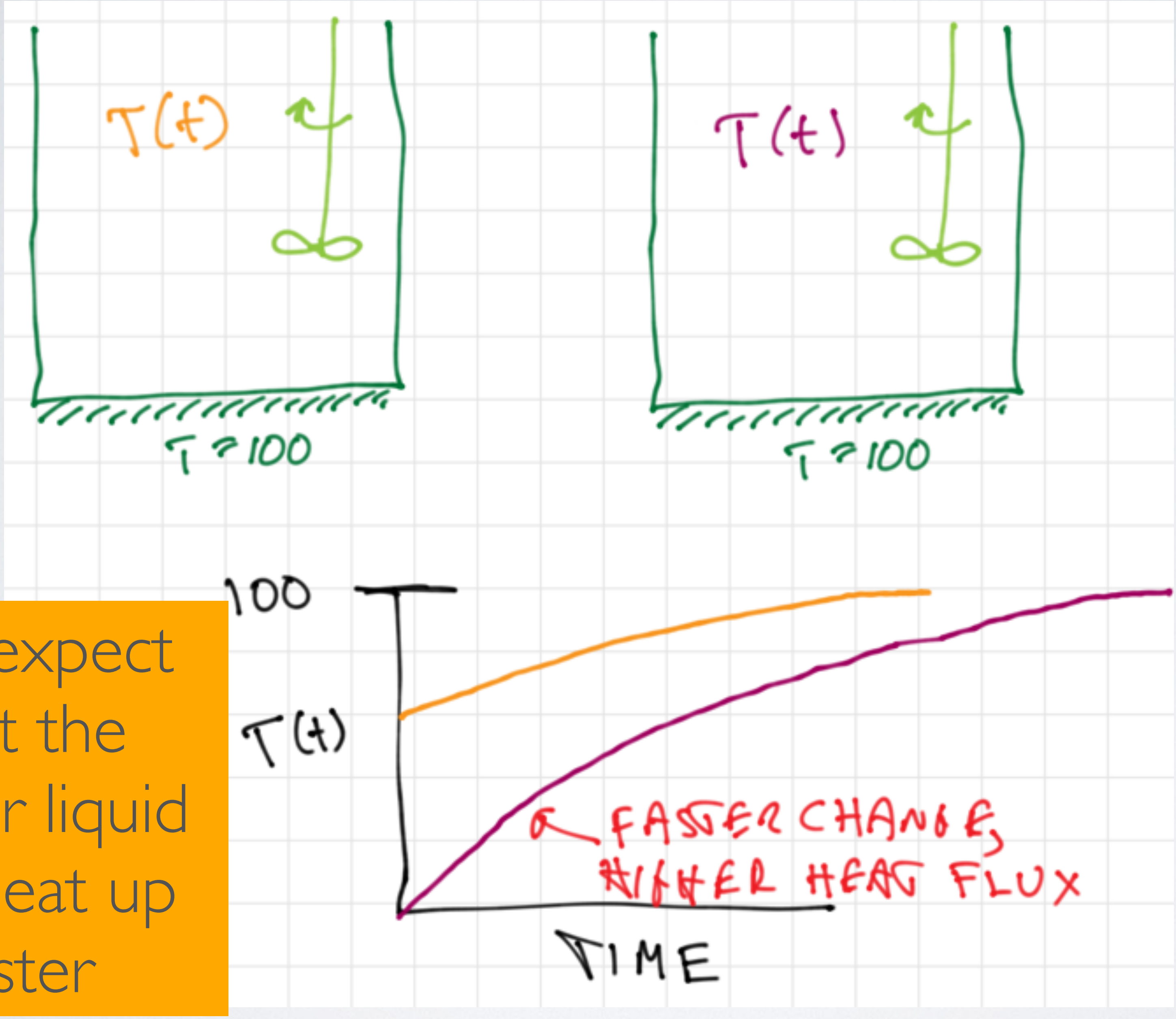
- Will some intuition allow us to gain insight into the most basic aspects of transport phenomena?

- We focus on the rate of change of concentration and temperature

    - For this simple set of problems, we don't consider the profile of concentration or temperature close to surfaces

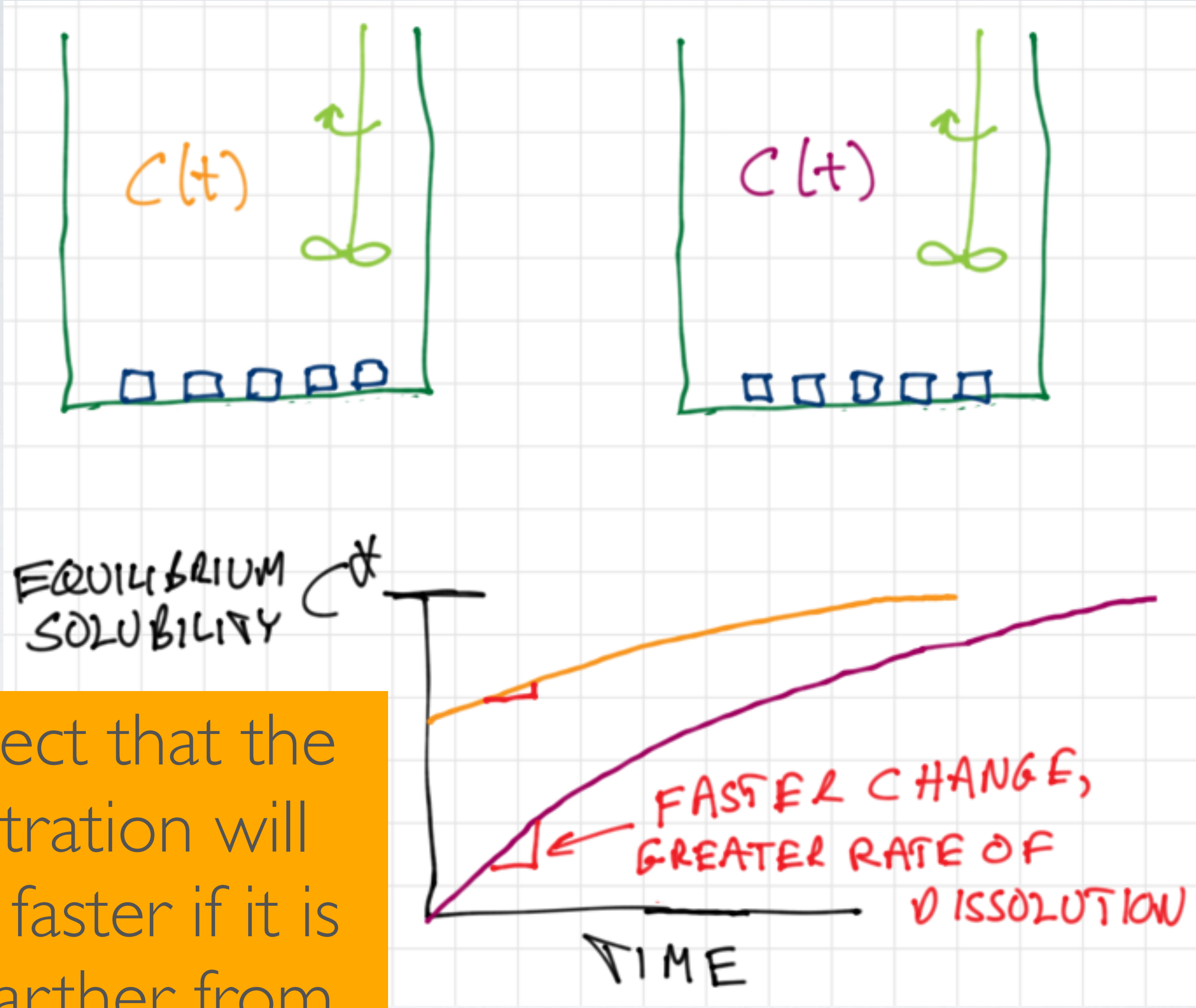
- Consider the following situations.

TEMPERATURE RISE IN A LIQUID



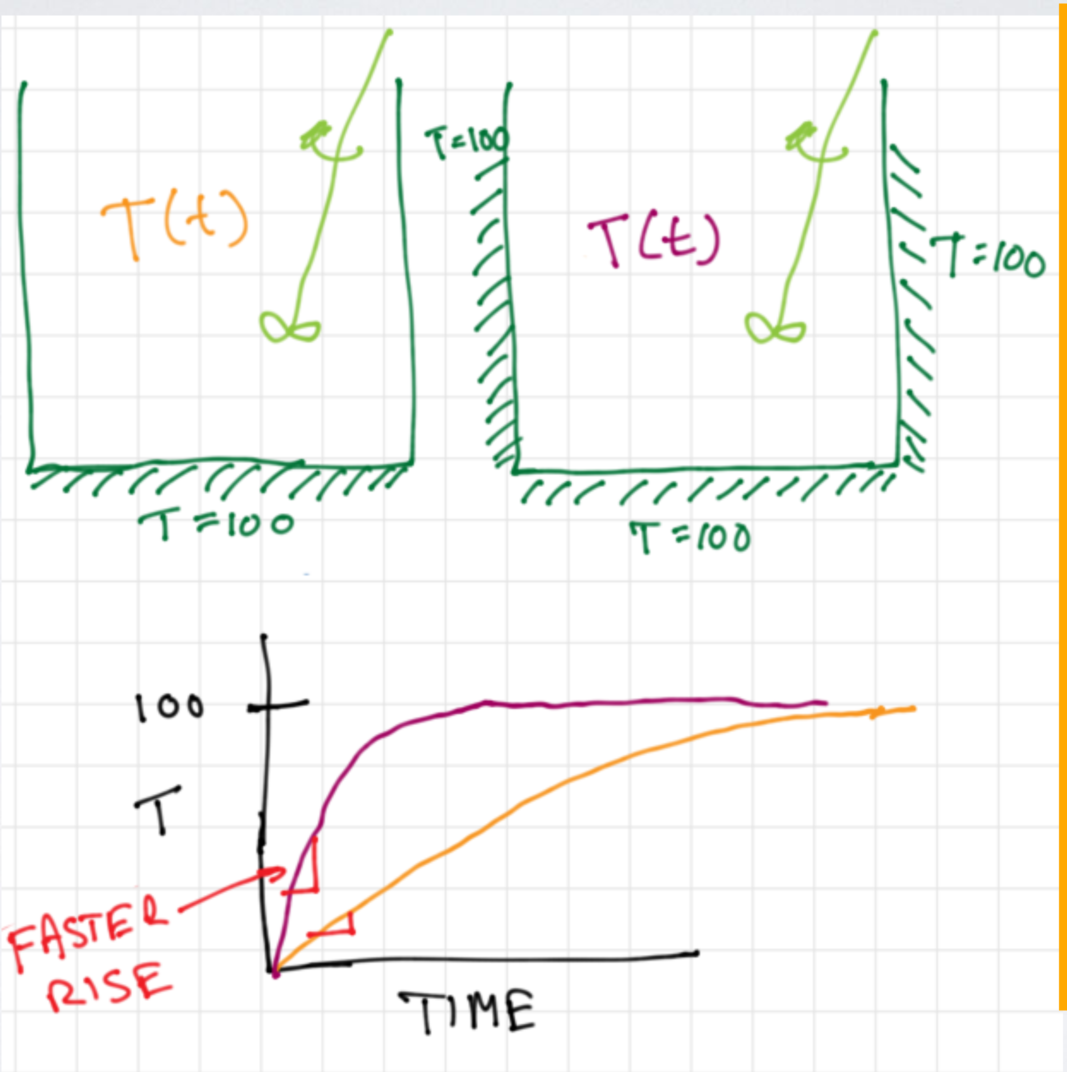
We expect that the cooler liquid will heat up faster

DISSOLUTION OF SOLID



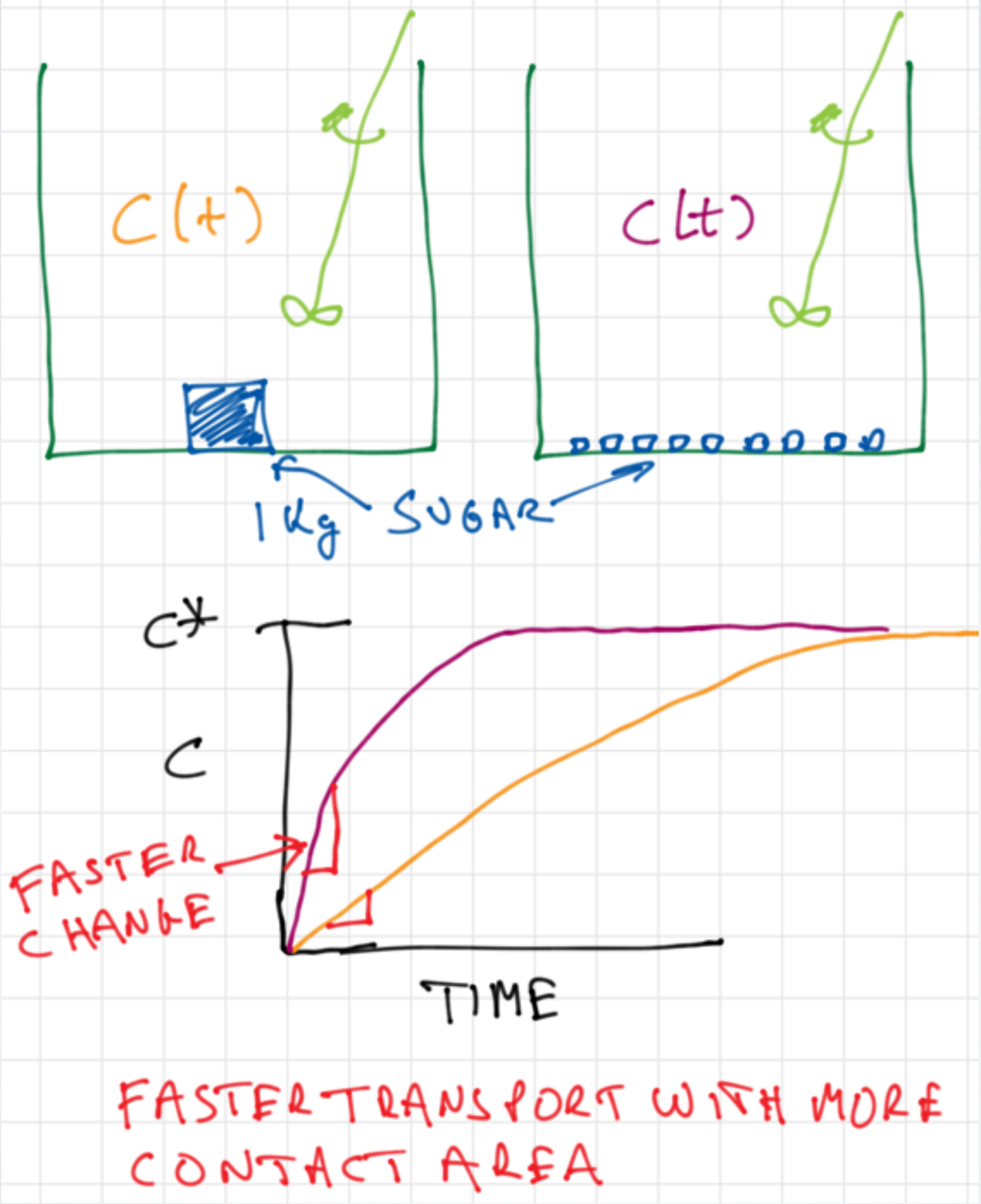
We expect that the concentration will increase faster if it is initially farther from equilibrium

TEMPERATURE RISE IN LIQUID



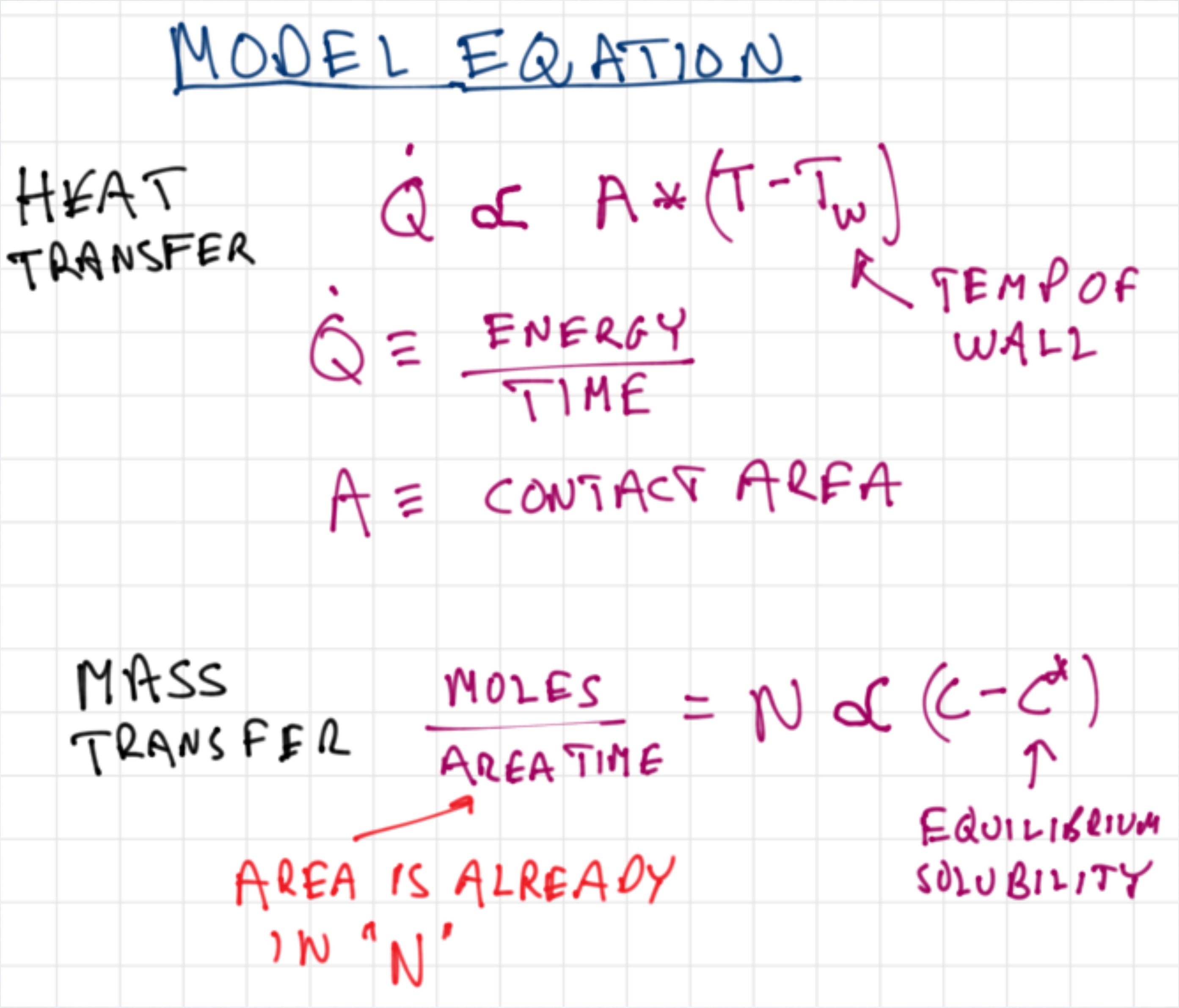
We expect that if there is more total contact area between hot surface and liquid, temperature will increase faster

DISSOLUTION OF SOLID



We expect that if there is more total contact area between solid and liquid, concentration will increase faster

HYPOTHESIZED EQUATION



MODEL EQATION

HEAT TRANSFER

$$\dot{Q} \propto A * (T - T_w)$$

TEMP OF WALL

$$\dot{Q} \equiv \frac{\text{ENERGY}}{\text{TIME}}$$

$A \equiv$ CONTACT AREA

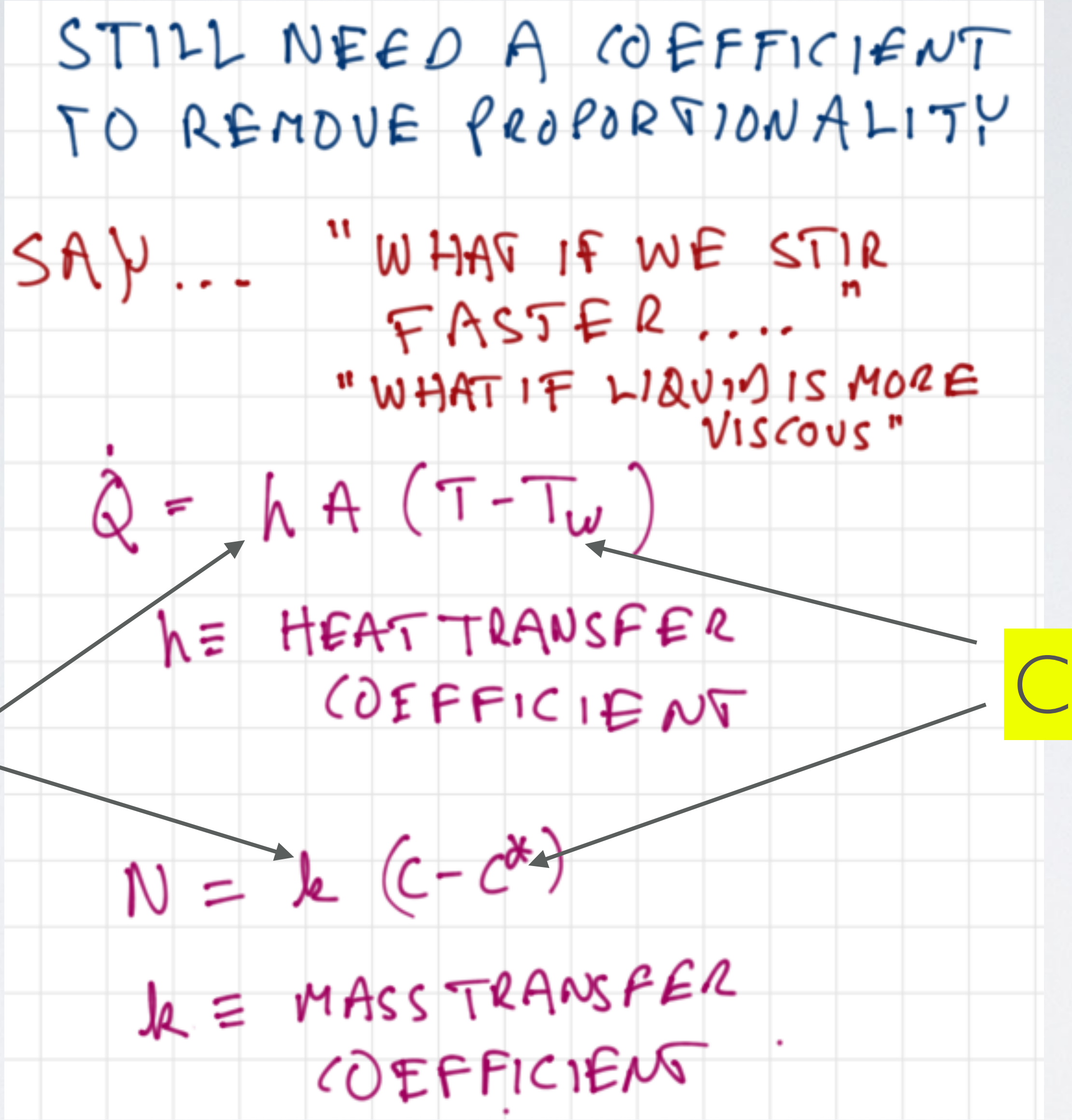
MASS TRANSFER

$$\frac{\text{MOLES}}{\text{AREA TIME}} = N \propto (C - C^*)$$

EQUILIBRIUM SOLUBILITY

AREA IS ALREADY IN "N"

“NEWTON’S LAW OF COOLING



STILL NEED A COEFFICIENT TO REMOVE PROPORTIONALITY

SAY... "WHAT IF WE STIR FASTER...."

"WHAT IF LIQUID IS MORE VISCOUS"

$$\dot{Q} = hA(T - T_w)$$

h ≡ HEAT TRANSFER COEFFICIENT

$$N = k(c - c^*)$$

k ≡ MASS TRANSFER COEFFICIENT.

CBE 30355, 30356, 30357

CBE 30367

“Greatest of all equations!”

RESULTING EQUATION!

- “Greatest of all” engineering equations!

$$N_i = \mathrm{k}\ (\mathrm{C} - \mathrm{C}^*)$$

- N is the flux, the flow of a chemical species (moles/time) per area.
  - k is the *mass transfer coefficient* that is determined by the degree of mixing and irregular flow in the fluid near the interface as well as the molecular diffusivity and viscosity (transport phenomena)
  - (C-C^*) is the concentration gradient, a straightforward simplification of the chemical potential gradient, (thermodynamics)

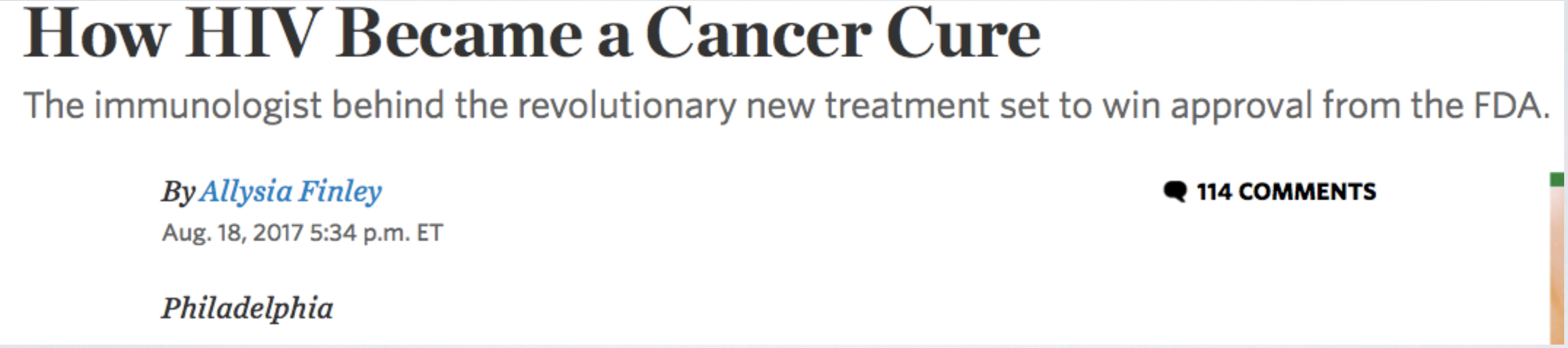
GREATEST OF ALL EQUATIONS: TWO PARTS

- Chemical thermodynamics tells us what this gradient (or algebraic driving force) will be and thus establishes <u>what</u> can happen
- Transport phenomena tells us <u>how fast</u> it is going to happen

MEET AND GREET!

- As in, find somebody you don’t know and introduce yourself

WSJ ARTICLE



How HIV Became a Cancer Cure

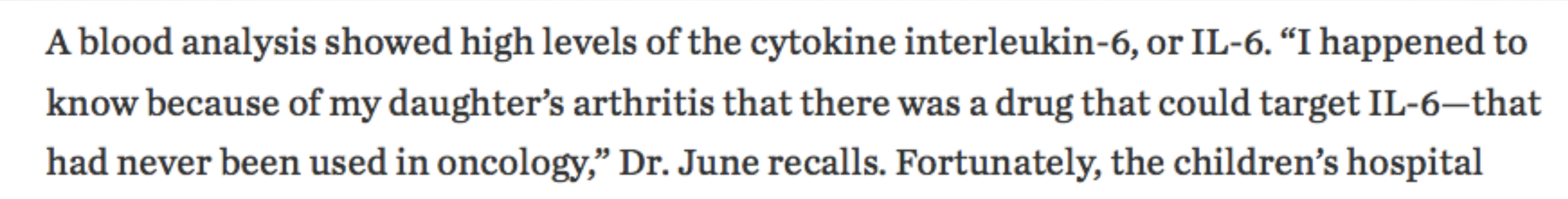
The immunologist behind the revolutionary new treatment set to win approval from the FDA.

By *Allysia Finley*

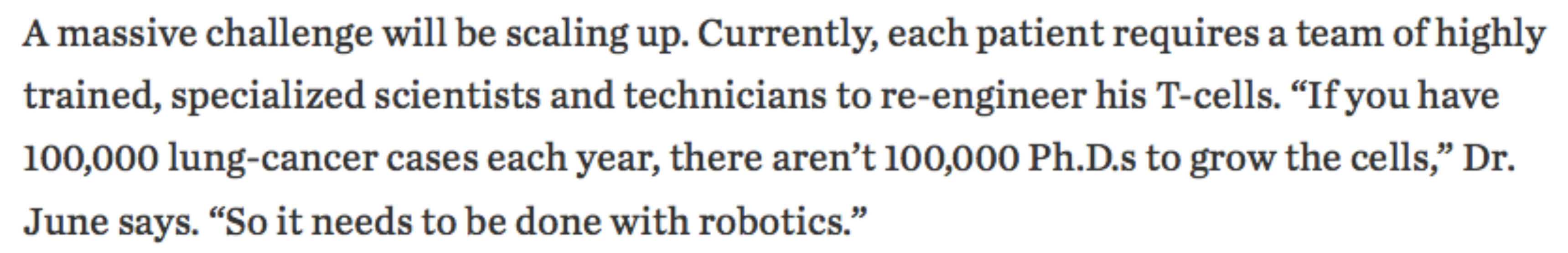
Aug. 18, 2017 5:34 p.m. ET

114 COMMENTS

Philadelphia



A blood analysis showed high levels of the cytokine interleukin-6, or IL-6. “I happened to know because of my daughter’s arthritis that there was a drug that could target IL-6—that had never been used in oncology,” Dr. June recalls. Fortunately, the children’s hospital



A massive challenge will be scaling up. Currently, each patient requires a team of highly trained, specialized scientists and technicians to re-engineer his T-cells. “If you have 100,000 lung-cancer cases each year, there aren’t 100,000 Ph.D.s to grow the cells,” Dr. June says. “So it needs to be done with robotics.”

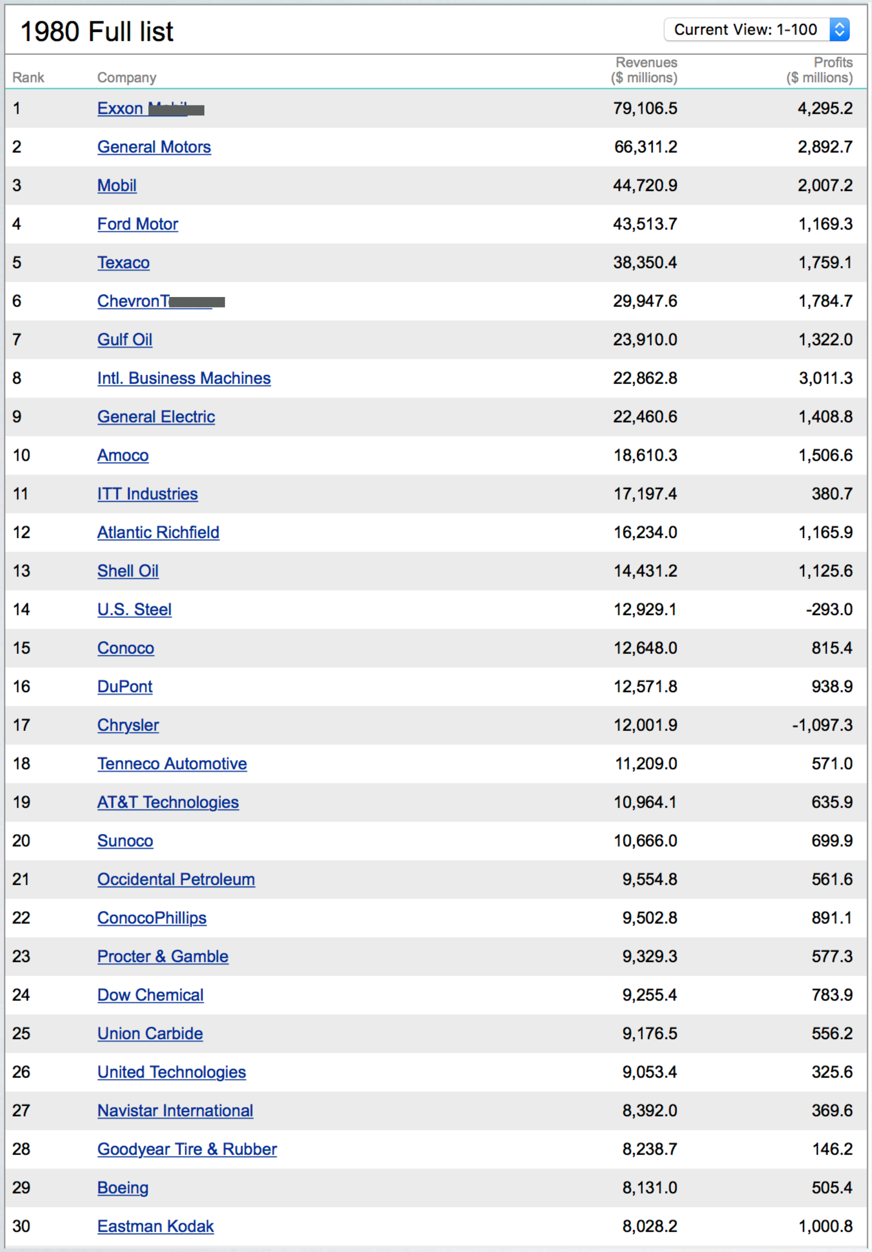
HANS HAUG
REACTOR SPECIALIST AT DUPONT

The more you know, the better engineer you will be!

WHY "BIO"

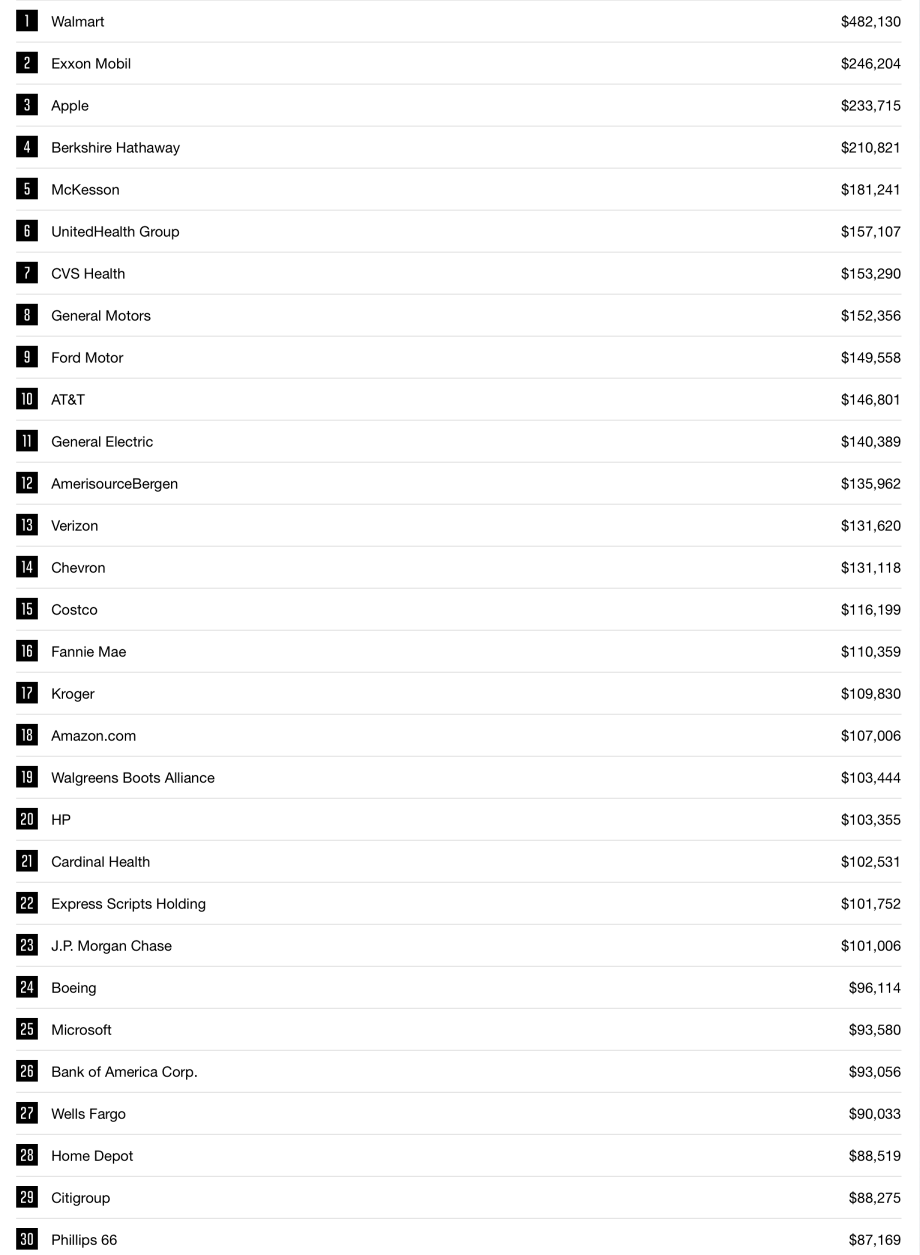
- Healthcare is an import issue for society
  - Engineers have not really made their mark yet.
- Interesting and possibly richer problems than if we just consider the chemical process industries
- Transformation of the chemical industry
  - We know how to make almost everything we need pretty well
    - Profitability is ~low…

FORTUNE "30", 1980 — 2016



1980 Full list

Rank	Company	Revenues ($ millions)	Profits ($ millions)
1	Exxon [redacted]	79,106.5	4,295.2
2	General Motors	66,311.2	2,892.7
3	Mobil	44,720.9	2,007.2
4	Ford Motor	43,513.7	1,169.3
5	Texaco	38,350.4	1,759.1
6	ChevronT[redacted]	29,947.6	1,784.7
7	Gulf Oil	23,910.0	1,322.0
8	Intl. Business Machines	22,862.8	3,011.3
9	General Electric	22,460.6	1,408.8
10	Amoco	18,610.3	1,506.6
11	ITT Industries	17,197.4	380.7
12	Atlantic Richfield	16,234.0	1,165.9
13	Shell Oil	14,431.2	1,125.6
14	U.S. Steel	12,929.1	-293.0
15	Conoco	12,648.0	815.4
16	DuPont	12,571.8	938.9
17	Chrysler	12,001.9	-1,097.3
18	Tenneco Automotive	11,209.0	571.0
19	AT&T Technologies	10,964.1	635.9
20	Sunoco	10,666.0	699.9
21	Occidental Petroleum	9,554.8	561.6
22	ConocoPhillips	9,502.8	891.1
23	Procter & Gamble	9,329.3	577.3
24	Dow Chemical	9,255.4	783.9
25	Union Carbide	9,176.5	556.2
26	United Technologies	9,053.4	325.6
27	Navistar International	8,392.0	369.6
28	Goodyear Tire & Rubber	8,238.7	146.2
29	Boeing	8,131.0	505.4
30	Eastman Kodak	8,028.2	1,000.8



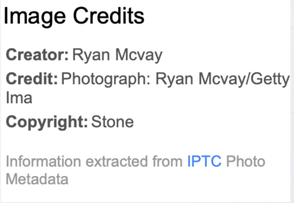
1	Walmart	$482,130
2	Exxon Mobil	$246,204
3	Apple	$233,715
4	Berkshire Hathaway	$210,821
5	McKesson	$181,241
6	UnitedHealth Group	$157,107
7	CVS Health	$153,290
8	General Motors	$152,356
9	Ford Motor	$149,558
10	AT&T	$146,801
11	General Electric	$140,389
12	AmerisourceBergen	$135,962
13	Verizon	$131,620
14	Chevron	$131,118
15	Costco	$116,199
16	Fannie Mae	$110,359
17	Kroger	$109,830
18	Amazon.com	$107,006
19	Walgreens Boots Alliance	$103,444
20	HP	$103,355
21	Cardinal Health	$102,531
22	Express Scripts Holding	$101,752
23	J.P. Morgan Chase	$101,006
24	Boeing	$96,114
25	Microsoft	$93,580
26	Bank of America Corp.	$93,056
27	Wells Fargo	$90,033
28	Home Depot	$88,519
29	Citigroup	$88,275
30	Phillips 66	$87,169

WHY: CBE 30357/ “BIO” ENGINEERING?

- > 100 years of “hard calculating”

from Wikipedia

- ~35 years with a soft start



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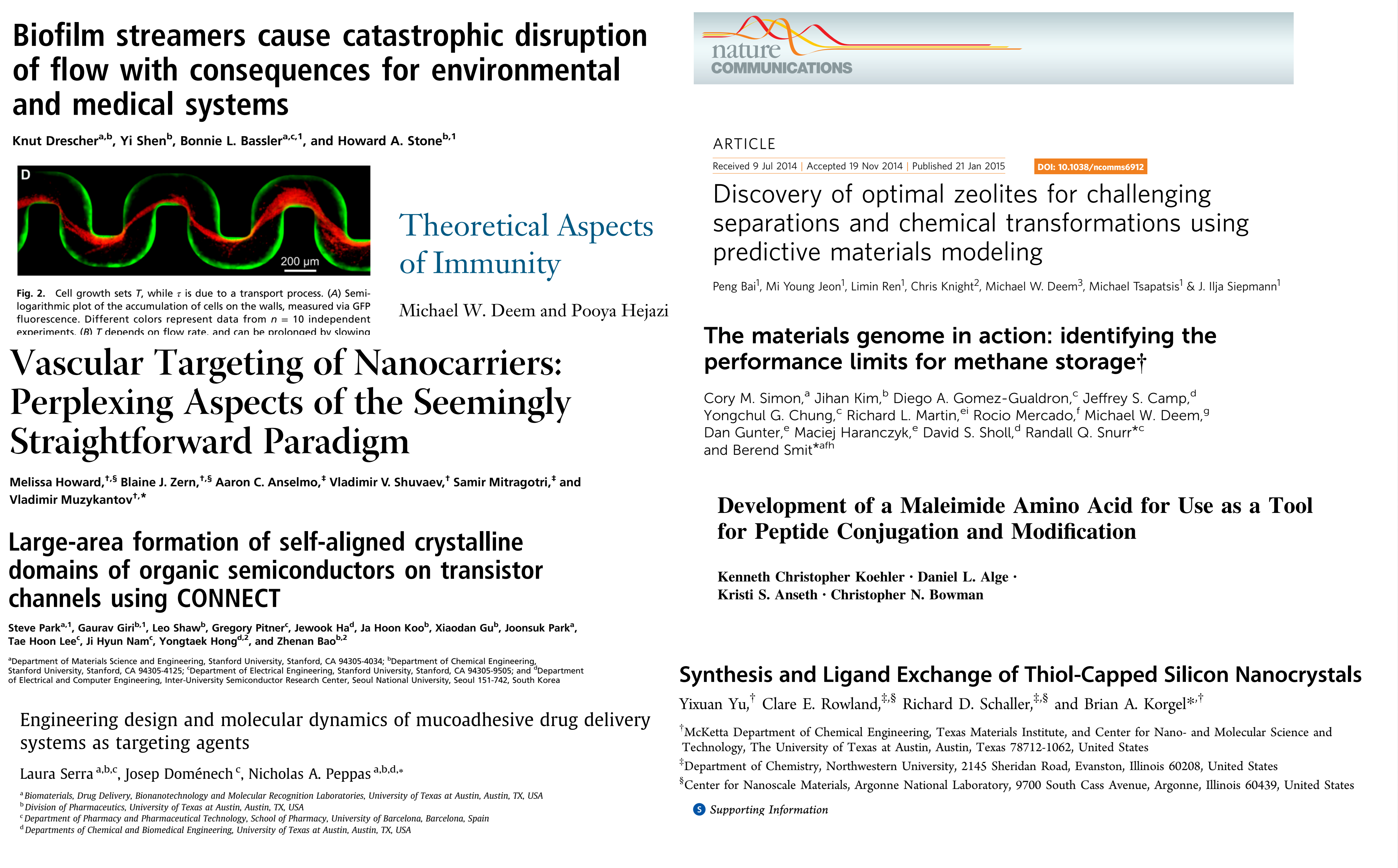
CHEMICAL ENGINEERING

- The **curricular major** of chemical engineering
- And
- the **intellectual foundation** of chemical engineering has benefitted from the <u>divergence</u> of the academic discipline from industrial practice
- The net result is that chemical engineering is perhaps most intellectually rich and academically broad academic major
  - (Potentially) we have more to say about a greater number of topics than anyone else!

RECENT RESEARCH BY CHEMICAL ENGINEERS



Biofilm streamers cause catastrophic disruption of flow with consequences for environmental and medical systems

Knut Drescher[a,b], Yi Shen[b], Bonnie L. Bassler[a,c,1], and Howard A. Stone[b,1]

Fig. 2. Cell growth sets T, while τ is due to a transport process. (*A*) Semi-logarithmic plot of the accumulation of cells on the walls, measured via GFP fluorescence. Different colors represent data from $n = 10$ independent experiments. (*B*) T depends on flow rate, and can be prolonged by slowing

Theoretical Aspects of Immunity

Michael W. Deem and Pooya Hejazi

Vascular Targeting of Nanocarriers: Perplexing Aspects of the Seemingly Straightforward Paradigm

Melissa Howard,[†,§] Blaine J. Zern,[†,§] Aaron C. Anselmo,[‡] Vladimir V. Shuvaev,[†] Samir Mitragotri,[‡] and Vladimir Muzykantov[†,*]

Large-area formation of self-aligned crystalline domains of organic semiconductors on transistor channels using CONNECT

Steve Park[a,1], Gaurav Giri[b,1], Leo Shaw[b], Gregory Pitner[c], Jewook Ha[d], Ja Hoon Koo[b], Xiaodan Gu[b], Joonsuk Park[a], Tae Hoon Lee[c], Ji Hyun Nam[c], Yongtaek Hong[d,2], and Zhenan Bao[b,2]

[a]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305-4034; [b]Department of Chemical Engineering, Stanford University, Stanford, CA 94305-4125; [c]Department of Electrical Engineering, Stanford University, Stanford, CA 94305-9505; and [d]Department of Electrical and Computer Engineering, Inter-University Semiconductor Research Center, Seoul National University, Seoul 151-742, South Korea

Engineering design and molecular dynamics of mucoadhesive drug delivery systems as targeting agents

Laura Serra [a,b,c], Josep Doménech [c], Nicholas A. Peppas [a,b,d,*]

[a] *Biomaterials, Drug Delivery, Bionanotechnology and Molecular Recognition Laboratories, University of Texas at Austin, Austin, TX, USA*
[b] *Division of Pharmaceutics, University of Texas at Austin, Austin, TX, USA*
[c] *Department of Pharmacy and Pharmaceutical Technology, School of Pharmacy, University of Barcelona, Barcelona, Spain*
[d] *Departments of Chemical and Biomedical Engineering, University of Texas at Austin, Austin, TX, USA*

ARTICLE

Received 9 Jul 2014 | Accepted 19 Nov 2014 | Published 21 Jan 2015 DOI: 10.1038/ncomms6912

Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling

Peng Bai[1], Mi Young Jeon[1], Limin Ren[1], Chris Knight[2], Michael W. Deem[3], Michael Tsapatsis[1] & J. Ilja Siepmann[1]

The materials genome in action: identifying the performance limits for methane storage†

Cory M. Simon,[a] Jihan Kim,[b] Diego A. Gomez-Gualdron,[c] Jeffrey S. Camp,[d] Yongchul G. Chung,[c] Richard L. Martin,[ei] Rocio Mercado,[f] Michael W. Deem,[g] Dan Gunter,[e] Maciej Haranczyk,[e] David S. Sholl,[d] Randall Q. Snurr*[c] and Berend Smit*[afh]

Development of a Maleimide Amino Acid for Use as a Tool for Peptide Conjugation and Modification

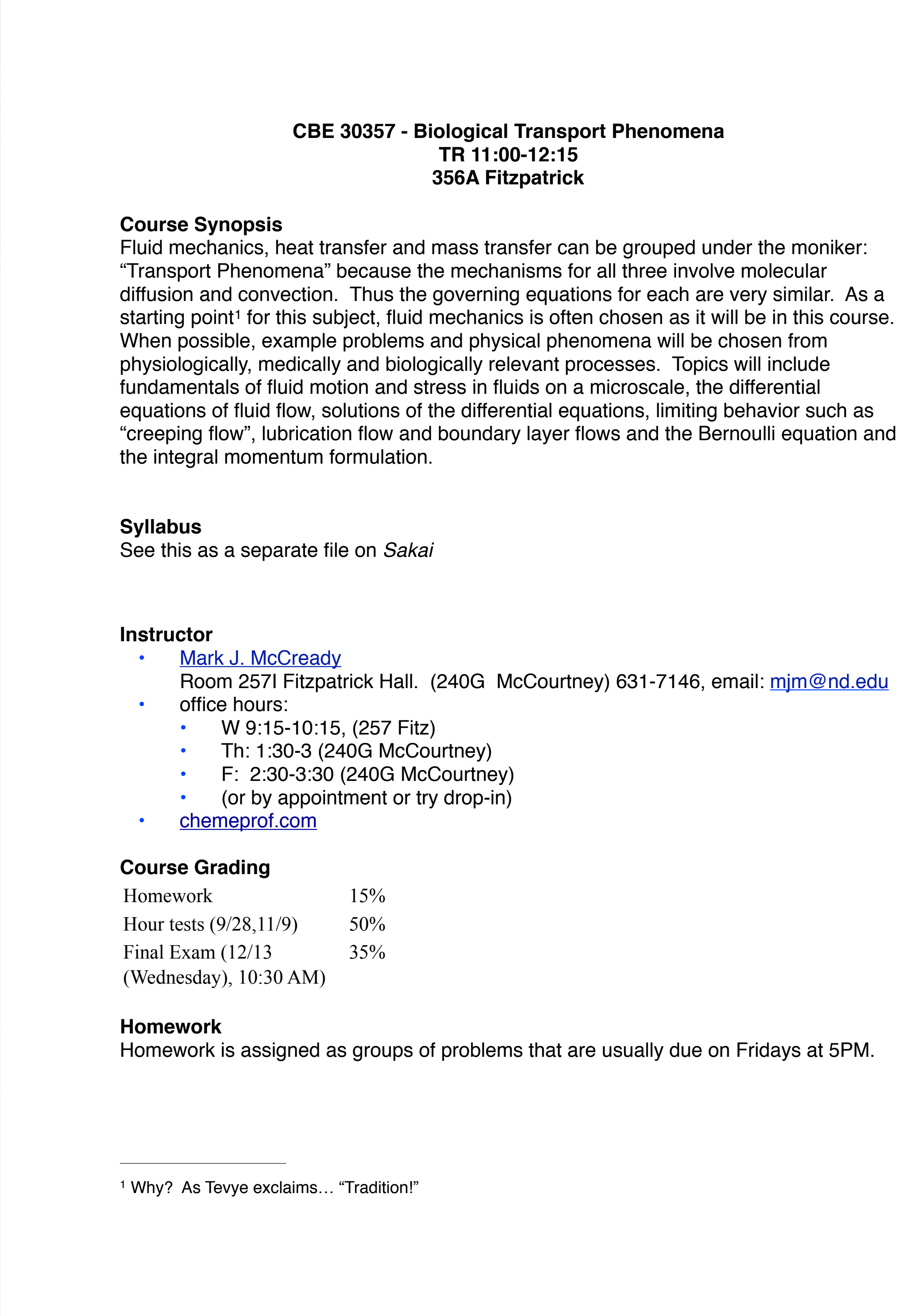
Kenneth Christopher Koehler · Daniel L. Alge · Kristi S. Anseth · Christopher N. Bowman

Synthesis and Ligand Exchange of Thiol-Capped Silicon Nanocrystals

Yixuan Yu,[†] Clare E. Rowland,[‡,§] Richard D. Schaller,[‡,§] and Brian A. Korgel*[,†]

[†]McKetta Department of Chemical Engineering, Texas Materials Institute, and Center for Nano- and Molecular Science and Technology, The University of Texas at Austin, Austin, Texas 78712-1062, United States
[‡]Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, United States
[§]Center for Nanoscale Materials, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States

S *Supporting Information*



CBE 30357 - Biological Transport Phenomena
TR 11:00-12:15
356A Fitzpatrick

Course Synopsis

Fluid mechanics, heat transfer and mass transfer can be grouped under the moniker: “Transport Phenomena” because the mechanisms for all three involve molecular diffusion and convection. Thus the governing equations for each are very similar. As a starting point[1] for this subject, fluid mechanics is often chosen as it will be in this course. When possible, example problems and physical phenomena will be chosen from physiologically, medically and biologically relevant processes. Topics will include fundamentals of fluid motion and stress in fluids on a microscale, the differential equations of fluid flow, solutions of the differential equations, limiting behavior such as “creeping flow”, lubrication flow and boundary layer flows and the Bernoulli equation and the integral momentum formulation.

Syllabus

See this as a separate file on *Sakai*

Instructor

- Mark J. McCready
  Room 257I Fitzpatrick Hall. (240G McCourtney) 631-7146, email: mjm@nd.edu
- office hours:
  - W 9:15-10:15, (257 Fitz)
  - Th: 1:30-3 (240G McCourtney)
  - F: 2:30-3:30 (240G McCourtney)
  - (or by appointment or try drop-in)
- chemeprof.com

Course Grading

Homework	15%
Hour tests (9/28,11/9)	50%
Final Exam (12/13 (Wednesday), 10:30 AM)	35%

Homework

Homework is assigned as groups of problems that are usually due on Fridays at 5PM.

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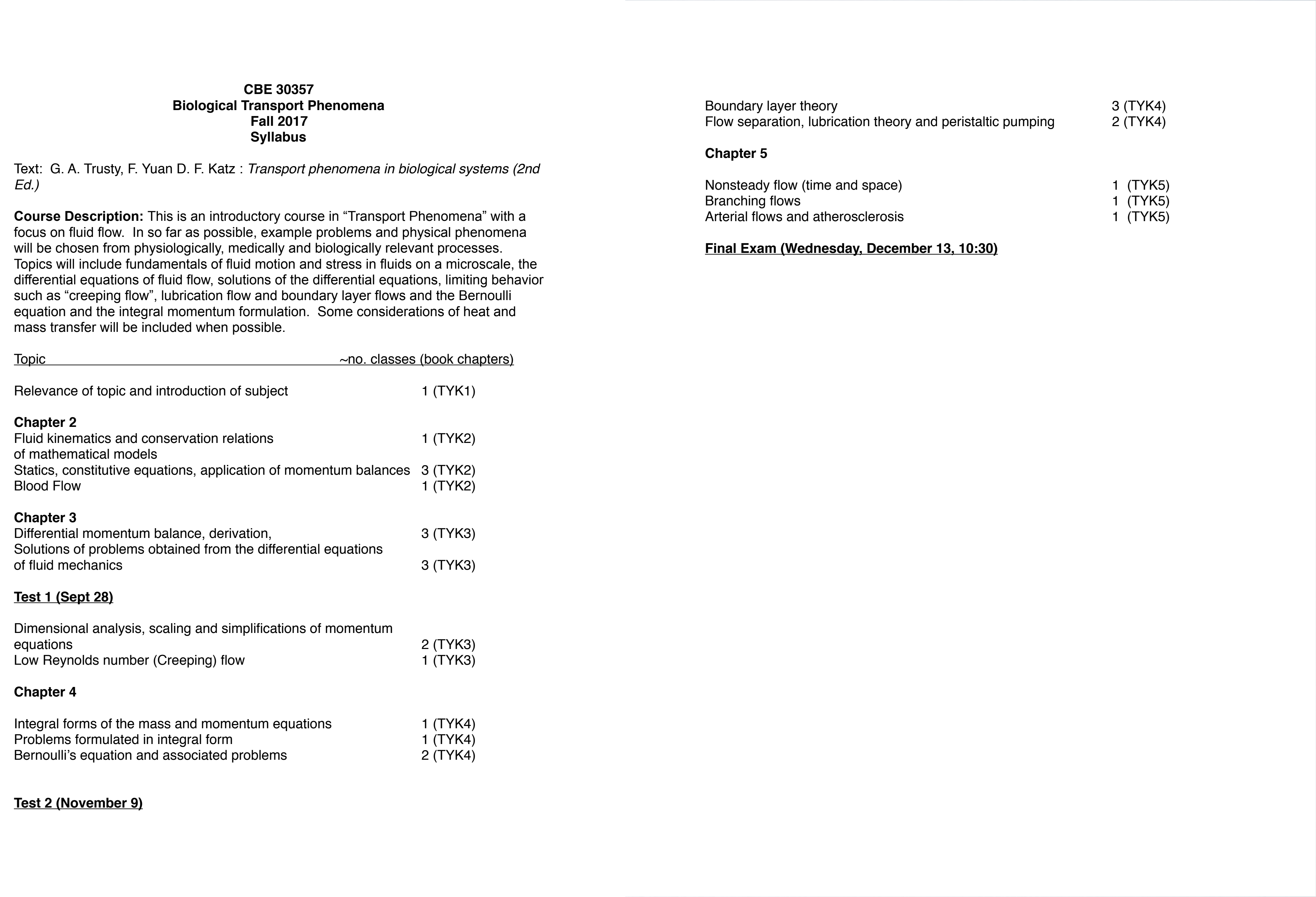
[1] Why? As Tevye exclaims… “Tradition!”



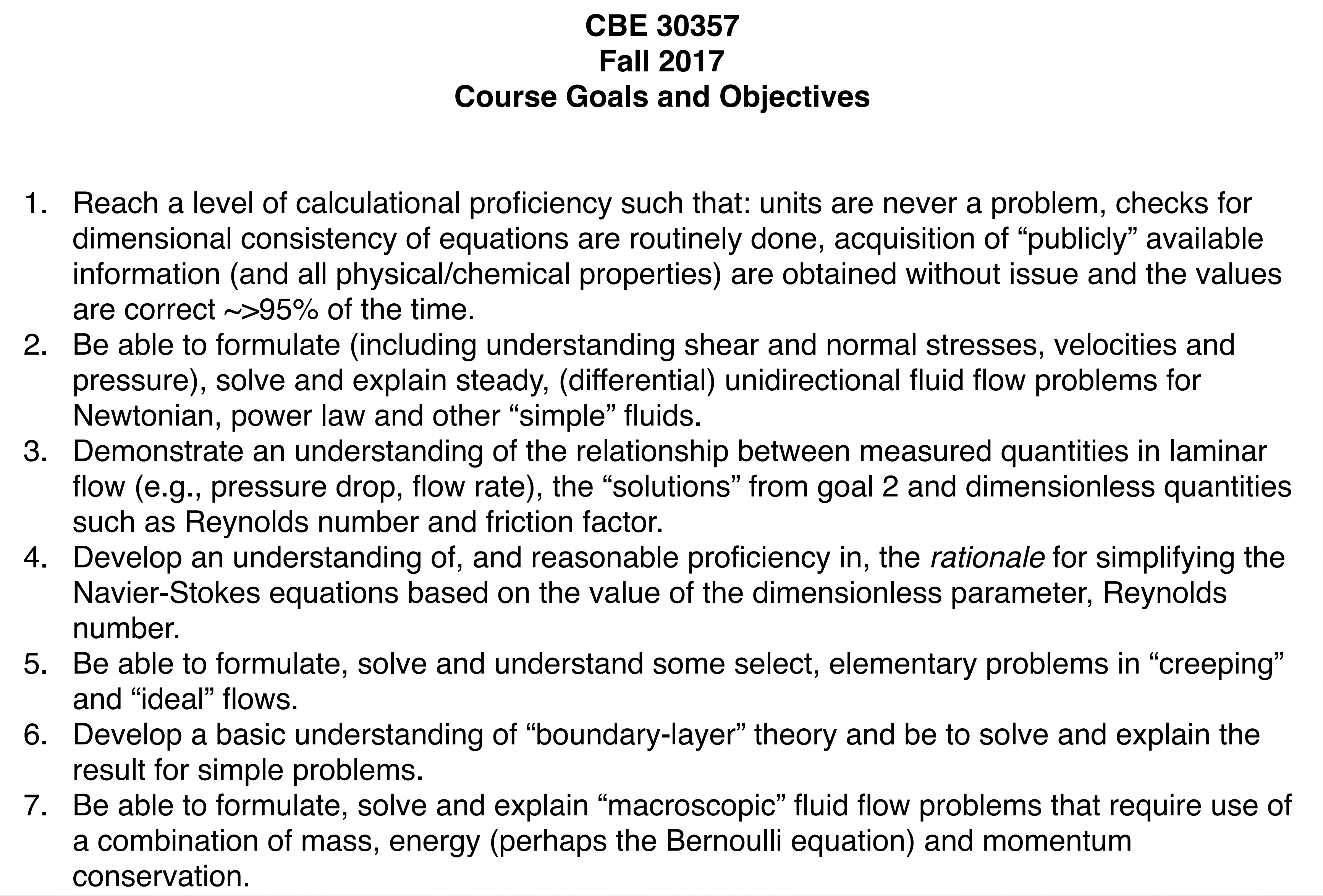
CBE 30357
Biological Transport Phenomena
Fall 2017
Syllabus

Text: G. A. Trusty, F. Yuan D. F. Katz : *Transport phenomena in biological systems (2nd Ed.)*

Course Description: This is an introductory course in “Transport Phenomena” with a focus on fluid flow. In so far as possible, example problems and physical phenomena will be chosen from physiologically, medically and biologically relevant processes. Topics will include fundamentals of fluid motion and stress in fluids on a microscale, the differential equations of fluid flow, solutions of the differential equations, limiting behavior such as “creeping flow”, lubrication flow and boundary layer flows and the Bernoulli equation and the integral momentum formulation. Some considerations of heat and mass transfer will be included when possible.

Topic	~no. classes (book chapters)
Relevance of topic and introduction of subject	1 (TYK1)
Chapter 2	
Fluid kinematics and conservation relations of mathematical models	1 (TYK2)
Statics, constitutive equations, application of momentum balances	3 (TYK2)
Blood Flow	1 (TYK2)
Chapter 3	
Differential momentum balance, derivation,	3 (TYK3)
Solutions of problems obtained from the differential equations of fluid mechanics	3 (TYK3)
Test 1 (Sept 28)	
Dimensional analysis, scaling and simplifications of momentum equations	2 (TYK3)
Low Reynolds number (Creeping) flow	1 (TYK3)
Chapter 4	
Integral forms of the mass and momentum equations	1 (TYK4)
Problems formulated in integral form	1 (TYK4)
Bernoulli’s equation and associated problems	2 (TYK4)
Test 2 (November 9)	
Boundary layer theory	3 (TYK4)
Flow separation, lubrication theory and peristaltic pumping	2 (TYK4)
Chapter 5	
Nonsteady flow (time and space)	1 (TYK5)
Branching flows	1 (TYK5)
Arterial flows and atherosclerosis	1 (TYK5)

Final Exam (Wednesday, December 13, 10:30)



CBE 30357
Fall 2017
Course Goals and Objectives

1. Reach a level of calculational proficiency such that: units are never a problem, checks for dimensional consistency of equations are routinely done, acquisition of “publicly” available information (and all physical/chemical properties) are obtained without issue and the values are correct ~>95% of the time.
2. Be able to formulate (including understanding shear and normal stresses, velocities and pressure), solve and explain steady, (differential) unidirectional fluid flow problems for Newtonian, power law and other “simple” fluids.
3. Demonstrate an understanding of the relationship between measured quantities in laminar flow (e.g., pressure drop, flow rate), the “solutions” from goal 2 and dimensionless quantities such as Reynolds number and friction factor.
4. Develop an understanding of, and reasonable proficiency in, the *rationale* for simplifying the Navier-Stokes equations based on the value of the dimensionless parameter, Reynolds number.
5. Be able to formulate, solve and understand some select, elementary problems in “creeping” and “ideal” flows.
6. Develop a basic understanding of “boundary-layer” theory and be to solve and explain the result for simple problems.
7. Be able to formulate, solve and explain “macroscopic” fluid flow problems that require use of a combination of mass, energy (perhaps the Bernoulli equation) and momentum conservation.

OVERVIEW

- This course brings in two completely new ideas
  - (at least to you)
  - Conservation of momentum (vector quantity)
  - Differential analysis — allows us to solve problems on any length scale
- (We could, but we won't do much analysis based on molecular concepts)
  - "Can't make money a molecule at a time!)
    - I have been saying this since the 1980's but strictly speaking… it is no longer true!