NOTRE DAME CHEMICAL ENGINEERING

Professors
Troy Vogel and Mark McCready

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ARE YOU A CHEMICAL ENGINEER?…. WE REALLY NEED YOUR HELP!

Mark J McCready

OUTLINE

- Some preliminary info
- What is special about chemical engineers.
- Some likely future contributions to society!
  - Energy
  - Healthcare
- My last try at what I thought was a clever slide!

Chemical Engineering **Class of 2021**

80 students from 25 states and 3 countries (Korea, Mexico, Panama)

2019 CLASS EMPLOYMENT DESTINATIONS

84.51°
AbbVie
Accenture
Apache Corporation
ARCCO/Murray
Beghou Consulting
Booz Allen Hamilton
Clarion Consulting
Clearsulting Analyst
Deloitte
Dow Chemical
Eli Lilly
Epic Systems
ExxonMobil
Fiat Chrysler Automobiles
Gates Corporation
GE Healthcare
Globalfoundries

Green Tweed and Co.
Javlyn Process Systems
Keyence Corp
Kymanox
McDermott International
McKinsey
P&G
PPG Manufacturing Development Program
Protiviti
PwC
Renaissance Lakewood, LLC
restor3d
Savannah River Nuclear Solutions
Siemens Healthcare
Ultracell LLC
Unilever
United States Steel Corporation
W.R. Grace & Co.

University of Chicago Medical School
University of Cincinnati Medical School
University of Washington - PhD Bioengineering
UC Berkeley - PhD in Chemical Engineering
UNC/NC State Grad School
Rice University (PhD)
Purdue University Graduate School
MSM program at ND
Brown University
Princeton University Research Associate
RPI (PhD)

volunteer (Glenmary Home Missionaries)
Navy Nuclear Power School
Marine Propulsion-Naval Nuclear Laboratory

OBSERVATION (TO STUDENTS)

- While some of you may for a large chemical or petroleum company where there are other chemical engineers also employed…

- You can see that most will be working where a great deal of your value to the company is what you know— that no one else in the room or building does.

CHEMICAL ENGINEERING

- Chemical understanding of matter and ability to apply quantitative analysis tools on scales from molecules to cubic meters
  - Molecular thermodynamics: Phase/chemical equilibrium
  - Comprehensive treatment of transport phenomena including chemical reactions
  - Analysis procedures that combine conservation and rate equations that can describe individual devices or complete process across all of these scales
- All of this can be applied beyond chemical process technology to the environment, physiological/living systems and various other industrial sectors.

CURRICULUM HIGHLIGHTS

CBE 20255, Intro to Chemical Engineering

MATH 30650, Differential Equations
CHEM 30333, Analytical Chem
CHEM 31333, Analytical Chem Lab
CBE 30367 Thermodynamics II
CBE 30361, Materials
CBE 30355, Transport Phenomena I or CBE 30357, Biotransport

CBE Elective
CBE 41459, Chem Eng Lab II or CBE 41910, Bioengineering Lab
CBE 40443, Separation Process
CBE 40445, Chemical Reaction Engineering

MATH 20580, Linear Algebra & ODE's
CHEM 20273, Organic Chemistry II
Arts and Letters Course
CBE 20258, Numerical and Statistical Analysis
CBE 20260, Thermodynamics

CHEM 30324, Physical Chemistry
CBE 30356, Transport Phenomena II
CBE 30338, Chemical Process Control
CBE 31358, Chemical Engineering Lab I

CBE 40448, Process Design
Technical Elective*
Technical Elective*
CBE Elective

Topics of lasting and far reaching value!

1978 — UNIVERSITY OF DELAWARE
2020 — UNIVERSITY OF NOTRE DAME

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77-78 SPRING          EG79 BCHE CHEMICAL ENGINEERING
AS M  403 ADV CALCULUS FOR APPLICATIONS     3 P   3  0
AS PSY301 PERSONALITY                       3 A   3 12
EG CHE332 CHEMICAL ENG
EG CHE342 HEAT AND MAS
EG CHE345 CHEMICAL ENG
   SEMESTER:          15
   CUMULATIVE:       109
   ACADEMIC STATUS: DEA
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absolutely on-point abstract for project report!

Data by Peter Giannini, Elise Weldon, ...

Second
CHEM
CBE 30
CBE 30
CBE 31
Arts an

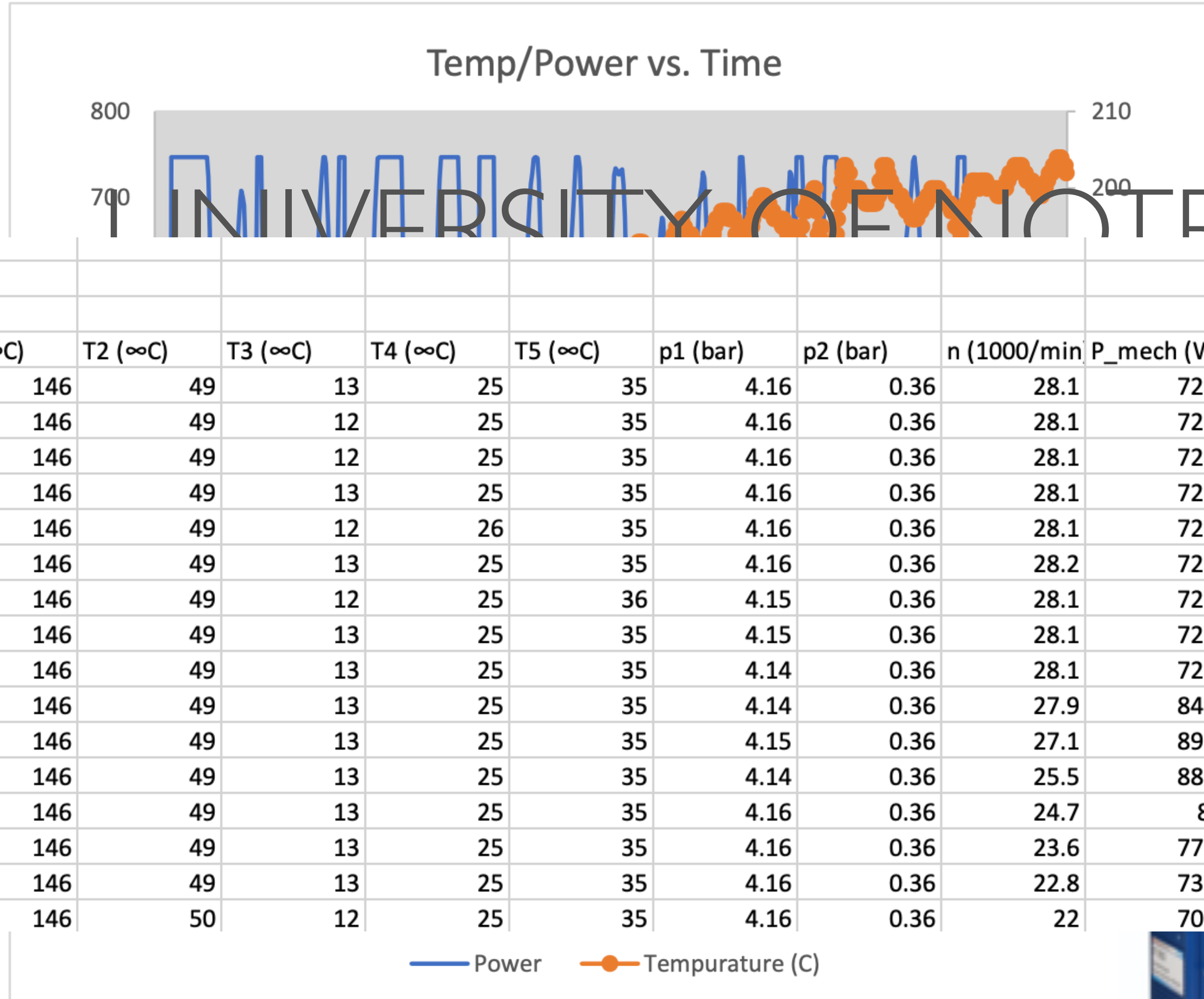
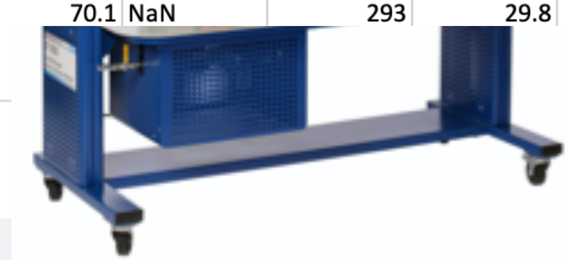


Figure 11. Water Temperature Change Response to the Superheater

turbine test

Time	T1 (∞C)	T2 (∞C)	T3 (∞C)	T4 (∞C)	T5 (∞C)	p1 (bar)	p2 (bar)	n (1000/min	P_mech (W)	F1 (ml/min)	F2 (l/h)	M (Nmm)
1/29/2020 2	146	49	13	25	35	4.16	0.36	28.1	72.2	NaN	289	24.5
1/29/2020 2	146	49	12	25	35	4.16	0.36	28.1	72.3	NaN	290	24.6
1/29/2020 2	146	49	12	25	35	4.16	0.36	28.1	72.5	NaN	287	24.6
1/29/2020 2	146	49	13	25	35	4.16	0.36	28.1	72.4	NaN	295	24.5
1/29/2020 2	146	49	12	26	35	4.16	0.36	28.1	72.4	NaN	300	24.6
1/29/2020 2	146	49	13	25	35	4.16	0.36	28.2	72.4	NaN	301	24.6
1/29/2020 2	146	49	12	25	36	4.15	0.36	28.1	72.4	NaN	292	24.5
1/29/2020 2	146	49	13	25	35	4.15	0.36	28.1	72.6	NaN	295	24.5
1/29/2020 2	146	49	13	25	35	4.14	0.36	28.1	72.6	NaN	295	26.8
1/29/2020 2	146	49	13	25	35	4.14	0.36	27.9	84.9	NaN	300	29.2
1/29/2020 2	146	49	13	25	35	4.15	0.36	27.1	89.2	NaN	295	30.1
1/29/2020 2	146	49	13	25	35	4.14	0.36	25.5	88.1	NaN	294	31.1
1/29/2020 2	146	49	13	25	35	4.16	0.36	24.7	82	NaN	291	30.9
1/29/2020 2	146	49	13	25	35	4.16	0.36	23.6	77.9	NaN	291	30.5
1/29/2020 2	146	49	13	25	35	4.16	0.36	22.8	73.6	NaN	296	30.1
1/29/2020 2	146	50	12	25	35	4.16	0.36	22	70.1	NaN	293	29.8



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I guess you don't have to use equations to cook ribs!

$$C_{102}H_{149}O_{38}N_{31} + H_2O \rightleftarrows C_{102}H_{151}O_{39}N_{31}$$

Collagen → Gelatin

COMPLETE MODEL

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} - \frac{\Delta H}{\rho C_p} A_0 e^{-E_a/RT}$$

CONDUCTION — COLLAGEN TO GELATIN REACTION

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - k C C_{col}$$

WATER DIFFUSION — HYDROLYSIS REACTION

x=0, L, L

INITIAL CONDITIONS

$$T(x,0) = 278\,K, \quad C(x,0) = .3$$

BOUNDARY CONDITIONS

$$\left.\frac{\partial T}{\partial x}\right|_0 = 0, \quad \left.\frac{\partial C}{\partial x}\right|_0 = 0$$ SYMMETRY

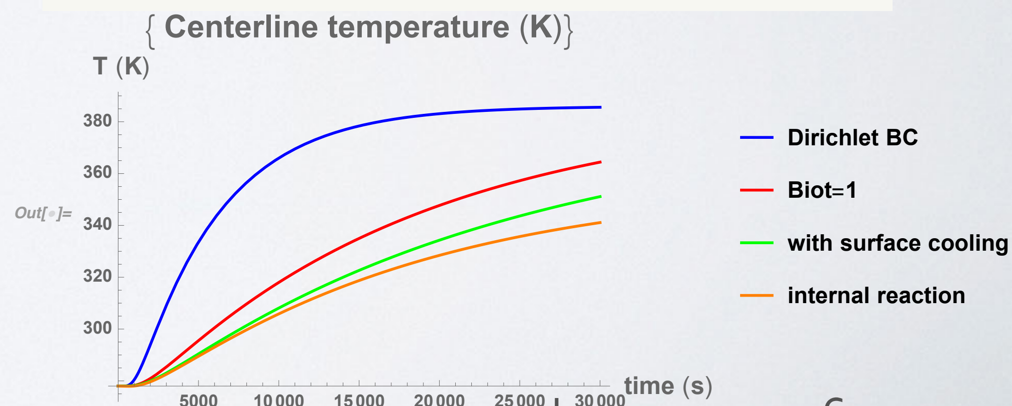
x=L)

$$-k\frac{\partial T}{\partial x} = h(T_L - T_\infty) - \Delta h_{vap}\, \rho \frac{\partial C}{\partial x}$$

CONDUCTION — NEWTON'S LAW OF COOLING — SURFACE EVAPORATIVE COOLING

$$-D\frac{\partial C}{\partial x} = k\left(\frac{P^{SAT}(T)}{P} C(L) - C_\infty\right)$$

DIFFUSION — SURFACE EVAPORATION



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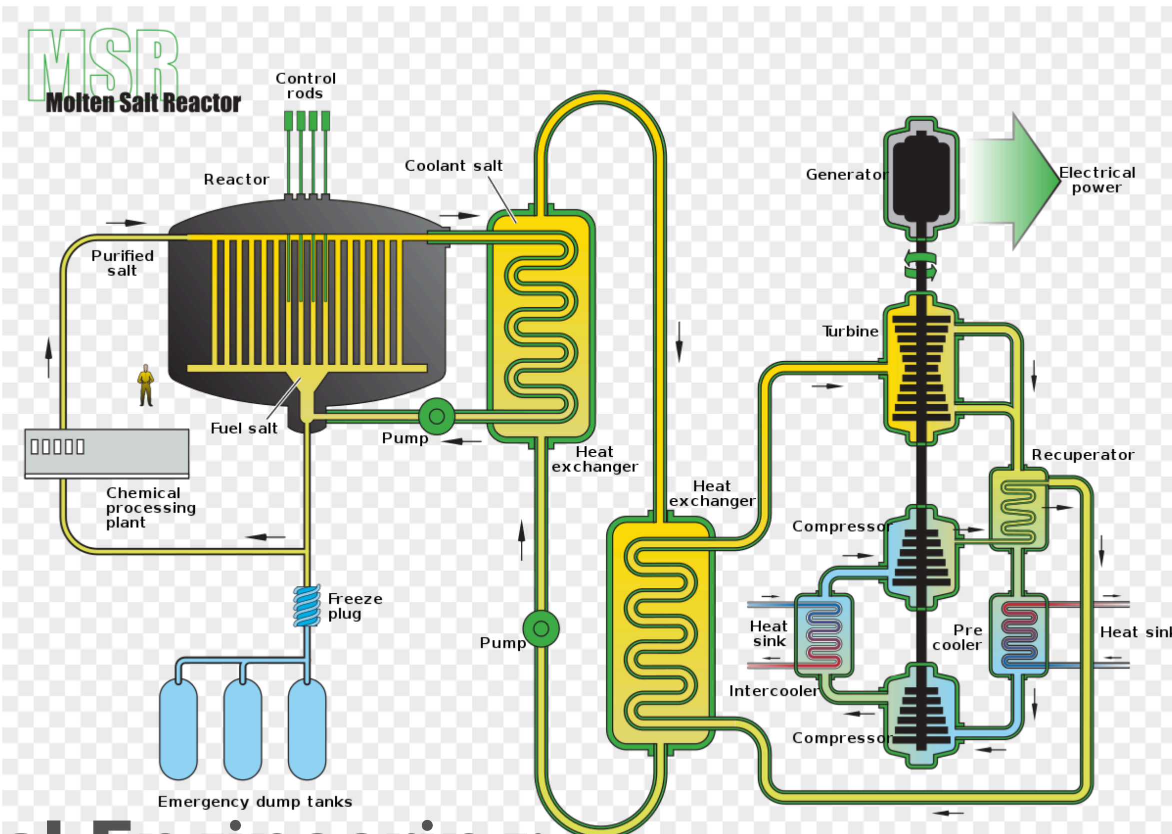
ENERGY

File:Molten Salt Reactor.svg

From Wikipedia, the free encyclopedia

Next generation nuclear power

File | File history | File usage | Global file usage | Metadata



Chemical Engineering:

- Molten salt: Thorium and Uranium are dissolved in salt mixture, need to understand this phase behavior, transport properties and materials of construction.

Prof Maginn works on some of these problems

ENERGY

- Maybe even CO_2 capture…

ENERGY: WHO WOULD HAVE THOUGHT!

Annual Review of Chemical and Biomolecular Engineering

The Energy Future

John Newman,[1] Christopher A. Bonino,[2] and James A. Trainham[3]

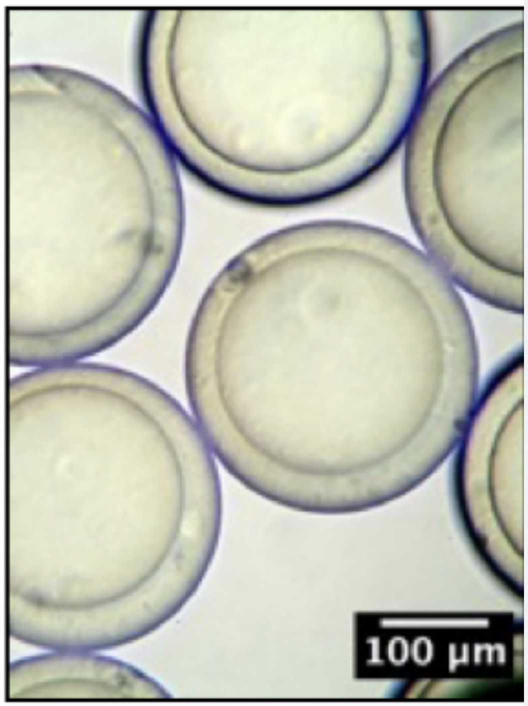
[1]Department of Ch... University of California, Berkeley, California 94720, U...

[2]... 27709, USA

[3]J...

Ionic liquid encapsulated in silicon based polymer

P2222 BnIm/H_2O in thiolene-Silica



Capturing CO2 might work for many processes

Diffusion and reaction in capsule control uptake

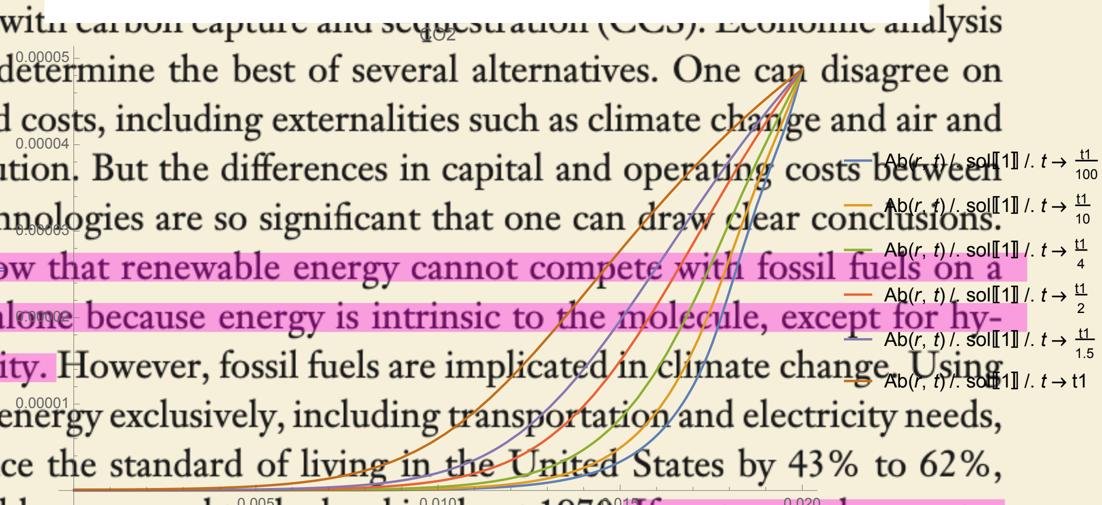
$$\frac{\partial \mathrm{Ab}(r,t)}{\partial t} = \frac{\alpha_1 \frac{\partial}{\partial r}\left(r^2 \frac{\partial \mathrm{Ab}(r,t)}{\partial r}\right)}{r^2} - k_{on}\,\mathrm{Ab}(r,t)\,\mathrm{Ag}(r,t) + k_{off}\,B(r,t),$$

$$\frac{\partial \mathrm{Ag}(r,t)}{\partial t} = \frac{\alpha_2 \frac{\partial}{\partial r}\left(r^2 \frac{\partial \mathrm{Ag}(r,t)}{\partial r}\right)}{r^2} - k_{on}\,\mathrm{Ab}(r,t)\,\mathrm{Ag}(r,t) + k_{off}\,B(r,t),$$

$$\frac{\partial B(r,t)}{\partial t} = k_{on}\,\mathrm{Ab}(r,t)\,\mathrm{Ag}(r,t) - k_{off}\,B(r,t)$$

Abstract

The foreseeab... tech-nologies and ... Re-newable ener... se of fossil fuels with carbon capture and sequestration (CCS). Economic analysis is used to determine the best of several alternatives. One can disagree on the detailed costs, including externalities such as climate change and air and water pollution. But the differences in capital and operating costs between known technologies are so significant that one can draw clear conclusions. Results show that renewable energy cannot compete with fossil fuels on a cost basis alone because energy is intrinsic to the molecule, except for hydroelectricity. However, fossil fuels are implicated in climate change. Using renewable energy exclusively, including transportation and electricity needs, could reduce the standard of living in the United States by 43% to 62%, which would correspond to the level in about 1970. If capture and sequester of CO_2 are implemented, the cost of fossil fuels will increase, but they beat renewable energy handily as an economic way to produce clean energy.



For 200 μm capsules: ~1 gmole/(m^3 s)

TRANSPORTATION

HEALTHCARE

A CALCULATION BEFORE SURGERY!

"Model-based control"

- Precise dosing for anesthesia
- Mass balances and reaction

Is this a way to possibly increase efficiency in healthcare?

Anesthesiology
1997; 87:884–99

Lippincott–Raven Publishers

Computer Simulation of the Effects of Alterations in Blood Flows and Body Composition on Thiopental Pharmacokinetics in Humans

D. Russell Wada, Ph.D.,* Sven Björkman, Ph.D.,† William F. Ebling, Ph.D.,‡ Hideyoshi Harashima, Ph.D.§, Sandra R. Harapat, B.A.,|| Donald R. Stanski, M.D.#

Background: **Understanding the influence of physiological variables on thiopental pharmacokinetics would enhance the scientific basis for the clinical usage of this anesthetic.**

Methods: **A physiological pharmacokinetic model for thiopental previously developed in rats was scaled to humans by substituting human values for tissue blood flows, tissue masses, and elimination clearance in place of respective rat values. The model was validated with published serum concentration data from 64 subjects. The model was simulated after intravenous thiopental administration, 250 mg, over 1 min, to predict arterial plasma concentrations under conditions of different cardiac outputs, degrees of obesity, gender, or age.**

Results: **The human pharmacokinetic model is characterized by a steady state volume of distribution of 2.2 l/kg, an elimination clearance of 0.22 l/min, and a terminal half-life of 9 h. Measured thiopental concentrations are predicted with an accuracy of 6 ± 37% (SD). Greater peak arterial concentrations are predicted in subjects with a low *versus* a high cardiac output (3.1 and 9.4 l/min), and in subjects who are lean *versus* obese (56 and 135 kg). Acutely, obesity influences concentrations because it affects cardiac output. Prolonged changes are due to differences in fat mass. Changes with gender and age are relatively minor.**

Conclusions: **The physiological pharmacokinetic model developed in rats predicts thiopental pharmacokinetics in humans. Differences in basal cardiac output may explain much of the variability in early thiopental disposition between subjects. (Key words: Anesthetics, intravenous: thiopental. Pharmacokinetics: thiopental.)**

Thiopental is an intravenous drug commonly used to induce general anesthesia. When clinical doses are administered, thiopental reversibly depresses brain activity and causes loss of consciousness within 10–20 s for a duration of 5–8 min.[1] Drug disposition plays an important role in onset and offset of thiopental's hypno-

Propofol

Propofol is a highly lipophilic hypnotic (octanol-water partition coefficient of 4300) and is the most commonly used hypnotic in the bariatric population. Like thiopental, propofol's kinetics are highly dependent on cardiac output (perfusion limited). In normal weight subjects, propofol has a high volume of distribution and clearance. It is primarily metabolized by the liver, however, its clearance exceeds hepatic blood flow, suggesting extra-hepatic metabolism. Propofol's high lipophillicity may suggest that the volume of distribution would be considerably higher in obese subjects compared to normal weight subjects, owing to their higher fat mass. In addition, the higher cardiac output seen in obese

CARDIOLOGY CALCULATION

Slide from CBE 30357

If you want to be really serious!

NAVIER–STOKES EQUATIONS FOR A NEWTONIAN FLUID WITH A CONSTANT VISCOSITY IN RECTANGULAR CARTESIAN (x, y, z) COORDINATES[a]

x component: $$\rho\left(\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = -\frac{\partial \mathcal{P}}{\partial x} + \eta\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right)$$

y component: $$\rho\left(\frac{\partial v_y}{\partial t} + v_x\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} + v_z\frac{\partial v_y}{\partial z}\right) = -\frac{\partial \mathcal{P}}{\partial y} + \eta\left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}\right)$$

z component: $$\rho\left(\frac{\partial v_z}{\partial t} + v_x\frac{\partial v_z}{\partial x} + v_y\frac{\partial v_z}{\partial y} + v_z\frac{\partial v_z}{\partial z}\right) = -\frac{\partial \mathcal{P}}{\partial z} + \eta\left(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}\right)$$

[a]The equations are written in terms of the equivalent pressure, $\mathcal{P}$.

where CO = cardiac output, HR = heart ... sure difference across the valve, and SEP ... tion period.

difference and linearly with area

AV_{TVI}

where AV = aortic valve flow velocity, LVOT = left

www.chemeprot.com

HEART BEAT ANALYSIS

- Claim: Specific features of ECG can predict heart health and even if someone is in pain!
- Chemical engineers are very good at data analysis — if we know what we are looking for and what it means… it is not "mining"

Instantaneous R-R interval

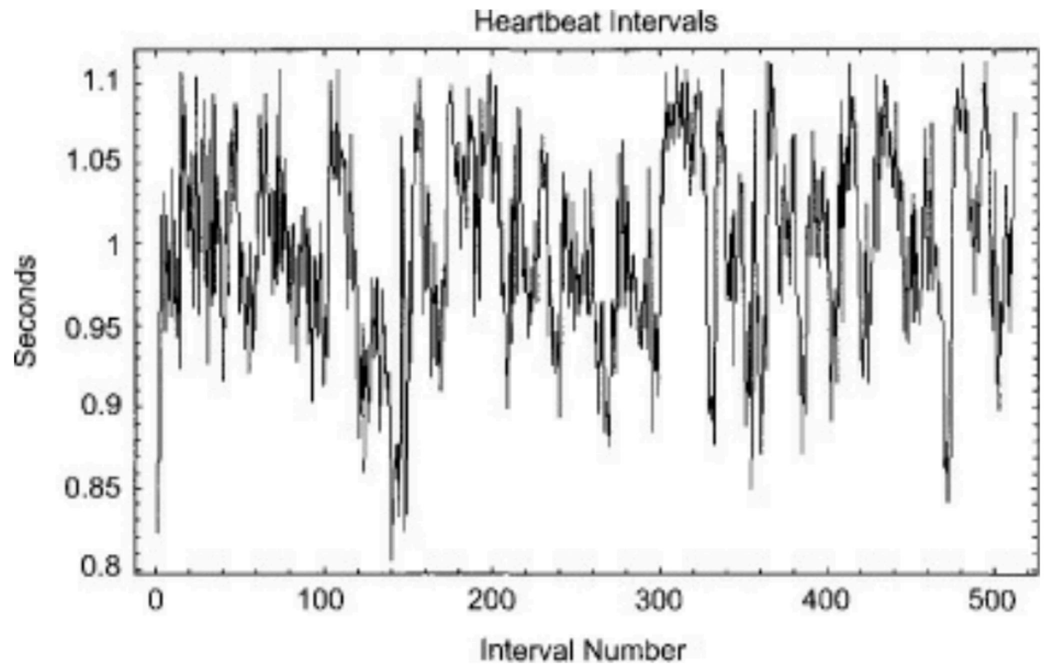


Fig. 5.6: The time series of heartbeat intervals of a healthy young adult male is shown. It is clear that the variation in the time interval between beats is relatively modest, but certainly not negligible.

My Apple Watch does something like this!

ANALYSIS OF INSTANTANEOUS HEART RATE

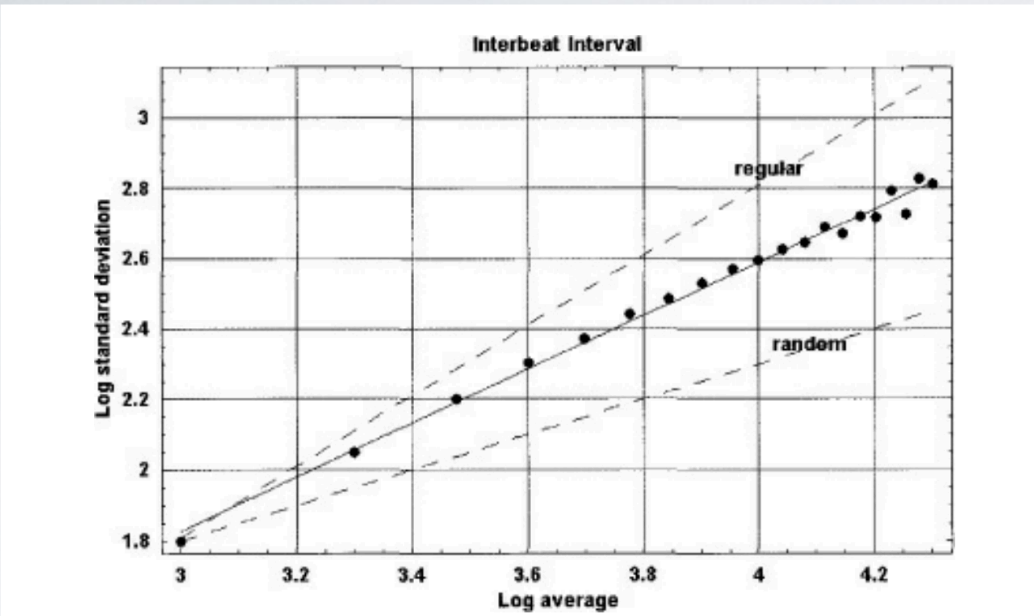


Fig. 5.7: The logarithm of the standard deviation is plotted versus the logarithm of the average value for the interbeat interval time series for a young adult male using different values of the aggregation number. The solid line is the best fit to the data points and yields a fractal dimension of $D = 1.24$ midway between the regular curve and the uncorrelated random curve.

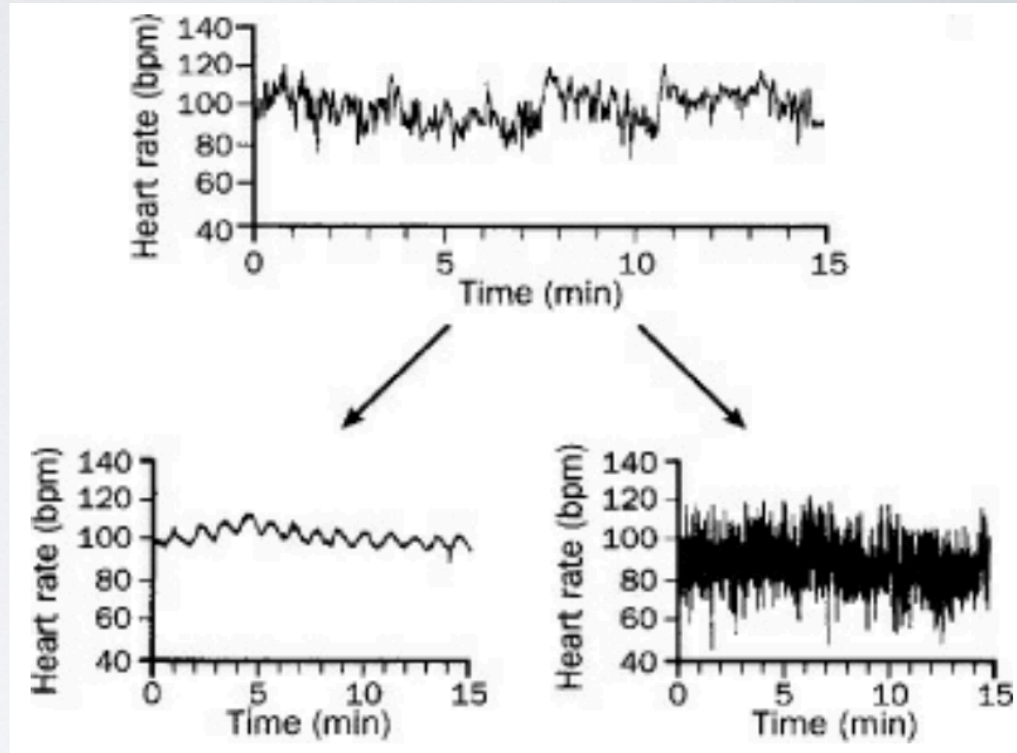


Fig. 7.2: A typical HRV time series with a fractal dimension in the interval $1.1 \le D \le 1.3$ is depicted by the upper curve. Two pathology branches emanate from this time series. The one on the left is congestive heart failure with fractal dimension approximately 1.0 and the one on the right is atrial fibrillation with fractal dimension approximately 1.5 (taken from Goldberger[58] with permission).

OK, BUT AN INDEX FOR PAIN

EJP
European Journal of Pain

REVIEW ARTICLE

Heart rate variability and experimentally induced pain in healthy adults: A systematic review

J. Koenig[1], M.N. Jarczok[2], R.J. Ellis[3], T.K. Hillecke[1], J.F. Thayer[4]

1 School of Therapeutic Sciences, SRH University, Heidelberg, Germany
2 Mannheim Institute of Public Health, Social and Preventive Medicine, Mannheim Medical Faculty, Heidelberg University, Mannheim, Germany
3 Department of Neurology, Beth Israel Deaconess Medical Center and Harvard Medical School, Boston, USA
4 Department of Psychology, The Ohio State University, Columbus, USA

Abstract

Background: Reactivity of the autonomic nervous system to experimental pain stimuli has been extensively studied using measures of heart rate and blood pressure. Heart rate variability (HRV) attempts to tease out the relative contributions of sympathetic and parasympathetic activity in the autonomic control of the heart and may therefore be more appropriate to investigate autonomic response to short-term nociceptive stimulation in detail. The current evidence on HRV and experimentally induced pain has not yet been synthesized within a systematic review.

Conclusion: HRV has several advantages compared to other measures of autonomic reactivity in studies investigating physiological response to nociceptive stimulation. Future studies should focus on comparisons between different methods of pain induction, interindividual variability in pain sensitivity by baseline autonomic activity, and the implications of both on the use of HRV within routine clinical evaluations.

EJA

Eur J Anaesthesiol 2016; **33:**118–125

ORIGINAL ARTICLE

Monitoring heart rate variability to assess experimentally induced pain using the analgesia nociception index

A randomised volunteer study

Gunnar Jess, Esther M. Pogatzki-Zahn, Peter K. Zahn and Christine H. Meyer-Frießem

BACKGROUND Pain assessment using a numerical rating scale (NRS) is considered good clinical practice, but objective assessment in noncommunicating patients is still a challenge. A potential solution is to monitor changes in heart rate variability transformed into the analgesia nociception index (ANI), that offers a noninvasive means of pain quantification.

CONCLUSION ANI did not allow a differentiation of painful, nonpainful or sham stimuli in alert volunteers. Therefore, ANI does not exclusively detect nociception, but may be modified by stress and emotion. Thus, we conclude that ANI is not a specific, robust measure for assessment of pain intensity.

BJA

British Journal of Anaesthesia, 123 (2): e312–e321 (2019)

doi: 10.1016/j.bja.2019.03.024
Advance Access Publication Date: 30 April 2019
Review Article

PERIOPERATIVE PAIN ASSESSMENT AND MANAGEMENT

Objective monitoring of nociception: a review of current commercial solutions

Thomas Ledowski[1,2,*]

[1]Anaesthesiology Unit, School of Medicine, University of Western Australia, Perth, Australia and [2]Dept. of Anaesthesia and Pain Medicine, Royal Perth Hospital, Perth, Australia

E-mail: Thomas.ledowski@health.wa.gov.au

NEEDED CONTRIBUTION BY CHEMICAL ENGINEERS

The New York Times

F.D.A. Approves First Gene-Altering Leukemia Treatment, Costing $475,000

A technician working with human cells belonging to cancer patients at Novartis Pharmaceuticals in Morris Plains, N.J. The Food and Drug Administration on Wednesday approved Novartis's gene therapy for leukemia, the first-ever treatment that alters a patient's own cells to fight cancer. Brent Stirton/Novartis Pharmaceuticals Corp., via Associated Press

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."

No, Actually, probably clever chemical engineering!

World Health Organization

JANUARY 27 2020, 12:01AM, THE TIMES

ACS Infectious Diseases

Viewpoint

pubs.acs.org/journal/aidcbc

The Challenge of Overcoming Antibiotic Resistance: An Adjuvant Approach?

Roberta J. Melander and Christian Melander*

Microbiome

Kirandeep Bhullar[1], Nicholas Waglechner[1], Andrew Pawlowski[1], Kalinka Koteva[1], Eric D. Banks[2],

Fast reaction, Da=1, Slow diffusion: diff = .1

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In[•]:= Show[intplot1, intplot2, intplot3, intplot4]
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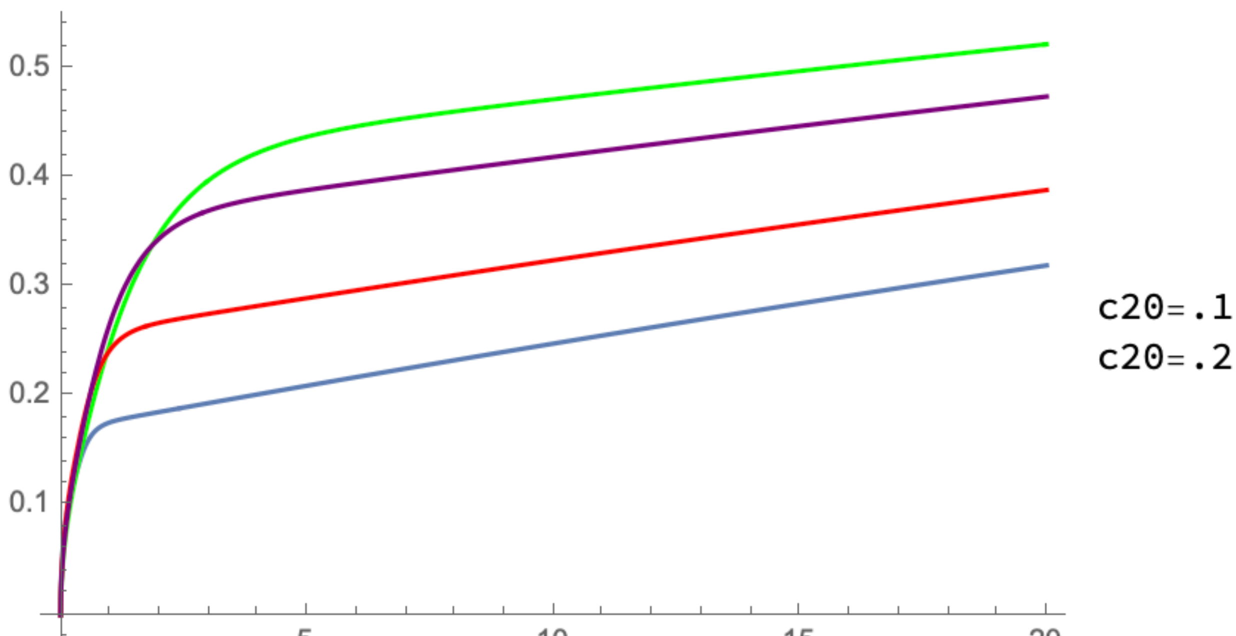
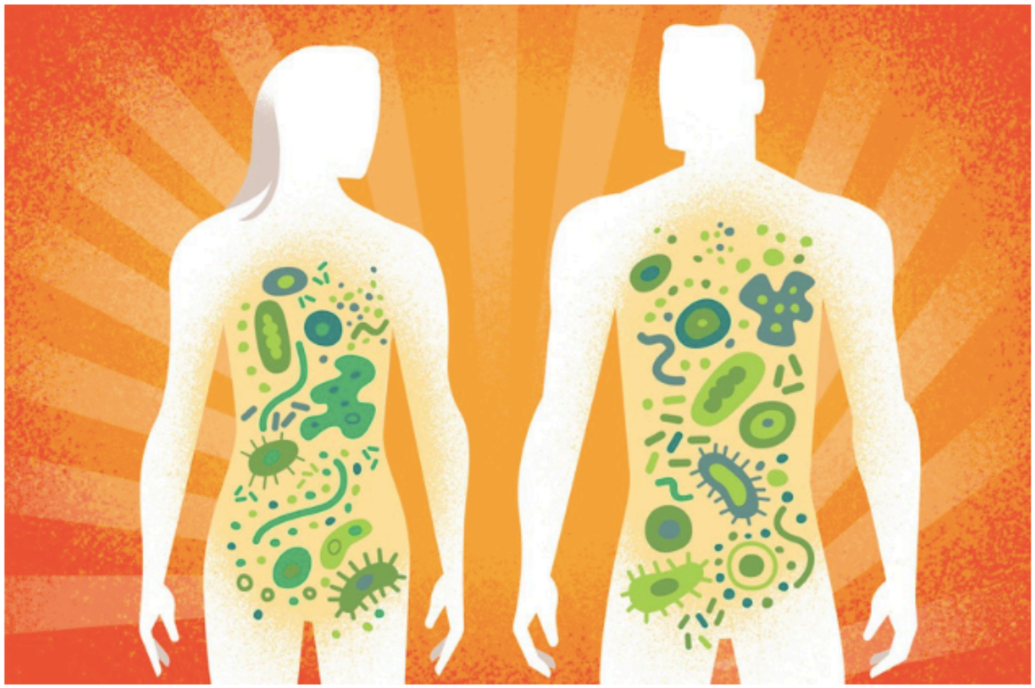


approaches to their identification.

CONTRIBUTION OF ENGINEERING

PERSONAL HEALTH

Unlocking the Secrets of the Microbiome



Paul Rogers

By Jane E. Brody

Nov. 6, 2017

105

Modern technology is making it possible for medical scientists to analyze inhabitants of our innards that most people probably would rather not know about. But the resulting information could one day save your health or even your life.

This is a "systems" problem as much as a biological problem.

How can we keep track of and interpret all of the biological data!

(academic) "TASSEL" LIST

- Go with your lab or HW group for breakfast or lunch with one of the faculty
- "voluntarily" take a deep academic experience e.g., figure out what the 2nd law really means, or what a normal viscous stress is or figure out why infinite domain transport problems have similarity variables naturally arising.
  - we can help!
- Ask a really perceptive question in class, or any question if you have never done it!
- Compliment a faculty member on a particularly good lecture

TASSEL LIST (CONTINUED)

- Explain (e.g.,) the utility of knowing the consequences of the first law of thermodynamics when, say, making green energy policy at ND, to a non-engineer !
- Read a publication written by one of the faculty members and discuss it with him or her over coffee.
- Attend a department research seminar or a similar seminar in another department
- Develop a fully-informed and well thought out position on an important world problem
- Make a *constructive* suggestion for course improvement on the CIF

SUMMARY

- Chemical engineers have knowledge and understanding that is both unique and useful far beyond chemical process technology
- We (as in you) are prepared to make seminal contributions to the future of society
  - — enjoy!