Chemical Engineering
as an
Academic Major and a Career

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Outline

Overview of chemical engineering

Impact of chemical engineers on society

A little about the curriculum

“Future” of Chemistry

Design innovations such as Princeton University’s Frick Chemistry Lab need to be matched by a radical rethink of priorities and teaching methods.

Let’s get practical

Chemistry needs an overhaul if it is to solve big global problems and advance fundamental understanding, say **George M. Whitesides** and **John Deutch**.

Chemistry is at the end of a century of expansion. In 1900, the chemical industry was in its infancy. The modern research university was still 50 years away, and the basic concepts of the field — the chemical bond, the laws of thermodynamics, theories of kinetics — were still being developed. In 2011, the industry is mature and fully embedded in society, and chemists have a good, semi-empirical grasp of many of the characteristics of molecules and reactions. Academic chemistry is established, and with its maturity has come an increasingly incurious and risk-averse attitude. So, what’s next?

‘Business as usual’ is not an option. To solve new problems, chemistry must be braver in its research choices and in how it organizes them. As it grew, academic chemistry splintered into many specialized subdisciplines such as organic synthesis, coordination chemistry and laser spectroscopy. This structure worked adequately for the relatively simple problems of the past century, but it will not work for the more complex problems of the next, such as global stewardship of natural resources. The field requires, and is undergoing, a fundamental change.

2011: YEAR OF CHEMISTRY
Celebrating the central science
nature.com/chemistry2011

Chemistry rests on three unequal legs: industry, academia and government. Of the three, only universities have the freedom and flexibility to take chemical science in new directions. Industry develops engineered, manufactured products; these should in principle solve societal problems, but must in practice be profitable. Under the short-term constraints of capitalism, industry has largely retreated from long-term research, and mostly focuses on incremental innovation. Government influences research through policy — how funding is allocated between fields, or tax credits for innovation, for instance — but influencing the direction of science is usually incidental to other political agendas. ▶

Nature Editorial
"Year of the Chemist"

- Chemistry should merge with chemical engineering!...
- Chemists need to better understand thermodynamics, mathematics, ...

We can start with a *Definition*

- **www.dictionary.com**

- chemical engineering **(km-kl nj-nîrng)**
- ***n.***

- **The branch of engineering that deals with the technology of large-scale chemical production and the manufacture of products through chemical processes.**
- ---
- chemical engineer ***n.***

Traditional chemical/petroleum industry

#Q-IND-284 • © Glen T. Brown/TSS 'XCV • rbair@aol.com

Traditional chemical/petroleum industry

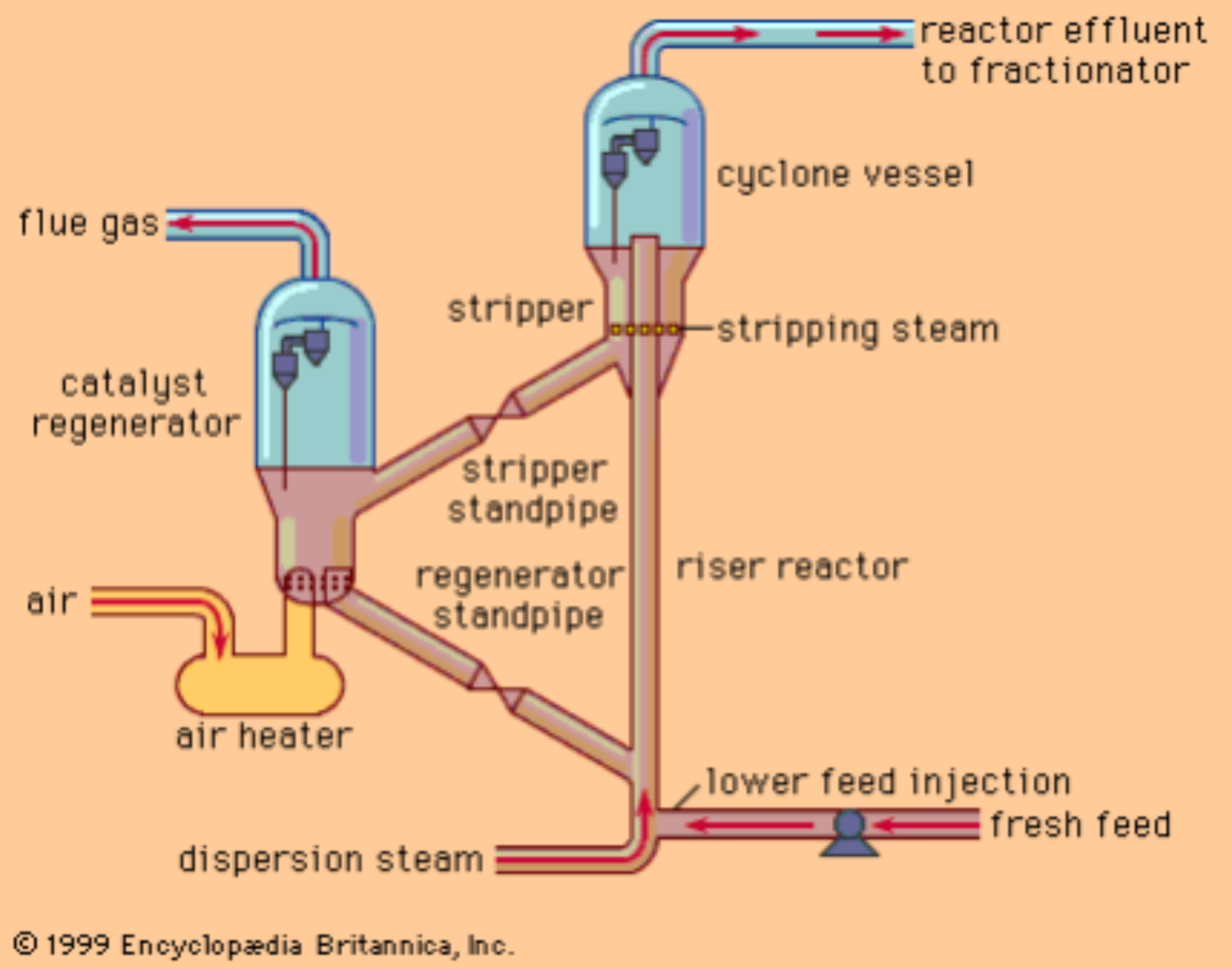
Large distillation tower

Traditional chemical/petroleum industry

Fluidized bed Catalytic Cracking unit

http://www.luboil.com/brief/brief.html

Cartoon of “Cat Cracker”



Chemical Reaction Engineering

- **What if the reactor is already built and we need to make more product?**
  - **How can we make reaction faster?**
  - **What controls how fast reactions occur?**
  - **Temperature**
- $K = A\ \mathrm{Exp}[-E_a/RT]$
  - **Arrhenius Expression**

What is chemical engineering?

- ***Chemical Engineering*** **originated with the need to transform raw materials into useful products through chemical reactions.**

- **The reactions were discovered by chemists starting in the 1600's and by the end of the 1800's, there was a need to produce large quantities of an ever increasing number of materials.**

- **The "scale-up" of a laboratory reaction (~grams) to a profitable commercial process 10^6 grams) is usually not a matter of just making bigger laboratory equipment (flasks, beaker and Bunsen burners).**

Primary characteristics of chemical engineers

- **Chemical** engineers understand matter in terms of its fundamental nature,
  - i.e., molecules,
  - can describe molecules or groups of molecules *quantitatively*
- They use *molecular understanding* to deal with processes involving chemical, biological and physical *transformations* of matter
- To effectively do this, they can answer the important questions necessary to bridge the gap from molecular sizes up to the dimensions of everyday life.

Major problems solved by chemical engineers

- "The American Institute of Chemical Engineers (AIChE) has identified the 10 most outstanding achievements of chemical engineering as being:
- 1.production of fissionable isotopes,
- 2.production of synthetic ammonia,
- 3.production of petrochemicals,
- 4.production of chemical fertilizers,
- 5.commercial-scale production of antibiotics,
- 6.establishment of the plastics industry,
- 7.establishment of the synthetic fibers industry
- 8.establishment of the synthetic rubber industry,
- 9.development of high-octane gasoline,
- 10.electrolytic production of aluminum.

Accomplishments

- "Chemical engineering is also involved in a major way in nuclear energy, medicine, materials science, food production, space, undersea exploration, and, above all, in energy production and the development of new sources of energy.

Key characteristics of Chemical Engineering

- Chemical Engineering has always remained close to its fundamental sciences: chemistry and biology and in fact seeks to drive these
- Beyond this chemical engineers have spent considerable time developing their own “science” that underlies much of what we do and cuts across many application areas

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Two central topics

- Thermodynamics: Phase equilibria
  - Explains the composition of gases, vapors, liquids and solids that are in continuous contact
    - Essential to understand for purification steps
- Transport Phenomena
  - Explains transport of chemical species on very small length scales (e.g., inside a catalyst particle, inside bone tissue)
  - Explains fluid flow and heat transfer on these scales as well

Soda Pop

- We discussed that soda pop fizzes when shaken, and not if not shaken, because shaking makes lots of small bubbles which serve as "surface area" for the CO_2 to go from the liquid to gas phase. The change in the equilibrium state is the same with or without shaking.
- The (approximate) phase equilibria equation is for this process is
- $x_i H_i = y_i P$
- where x_i is the liquid phase mole fraction, y_i is the gas phase mole fraction, H_i is the "Henry's Law" coefficient and P is total pressure. Inside the bottle, the CO_2 should be in equilibrium and shaking will have the minor effect of raising the temperature slightly.

Soda Pop

- Once the bottle is opened, the total pressure, P, drops slightly (~10%) and the mole fraction in the outside air (but not inside a bubble) also decreases. This change in equilibrium can lead to either a mild effect, if the surface area is limited, or a large effect (fizzing out of the bottle) if there is a large area available for interphase transport. The reason that the difference is so large is because phase change does not easily occur unless "interface" is already available. That is, a bubble will not spontaneously form in a liquid phase (this would be called *homogeneous nucleation*), unless the concentration driving force is much larger than would occur for a soda bottle. Note as an aside, the same effect occurs in boiling also where the vapor bubbles form at nucleation sites which are usually chips or scratches in the pan. Bubble nucleation at a solid site is called *heterogeneous nucleation*.

- The process of a chemical constituent is being transferred from one phase to another is called *mass transfer*. Chemical engineering processes are typically designed to make mass transfer as fast as possible by providing sufficient *transfer area* for mass transfer to occur.

Big impact areas

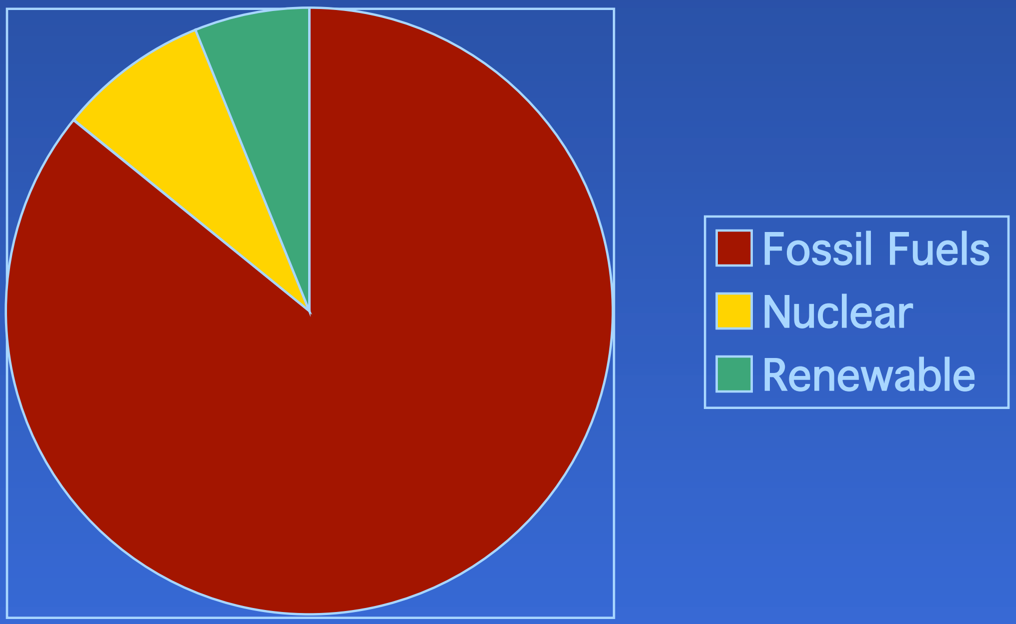
- Energy
- Healthcare

Big impact areas

- Energy

Energy!!

- **Where it comes from now!!**



Energy

- Even though there is no end in sight for carbon-based fuels
  - And there are chemical engineers trying to make this process as efficient and clean as possible
- this is inherently *un<u>Sustainable</u>*
  - At some point, particularly with increased world-wide usage, the remaining sources will become uneconomical or have too low an energy return.
  - CO_2 levels in the atmosphere will continue to increase and there is certainly a possibility of deleterious climate change.

Renewable Energy

Roles for chemical Engineers

- Solar cells
  - New materials, designed on a molecular scale, to capture energy more efficiently,
  - New processes to make these at lower cost.
- Biomass
  - Enabling technologies are needed
    - Wood, “grasses” to liquid fuels
      - Breaking down Cellulose to fermentable sugars is a combined chemistry and mass transfer challenge
      - Algae
- Geothermal
  - Design affordable systems to efficiently collect the energy
- Wind Power
  - Better materials: lighter and stiffer

Short(er) term alternatives

- Clean Coal technologies
  - High temperature gas separations
  - CO_2 sequestration
- Oil shale
  - How to produce useful fuel efficiently
    - Still have the CO2 problem
- Nuclear energy
  - Materials, process operation, waste issues remain important
- Increased efficiency
  - Energy growth is about 4% world wide
    - Great challenge for engineers: Gain >4% in efficiency worldwide!
    - Find and demonstrate where greatest payback will be!

Big impact areas

- Energy
- Healthcare

Tissue Engineering

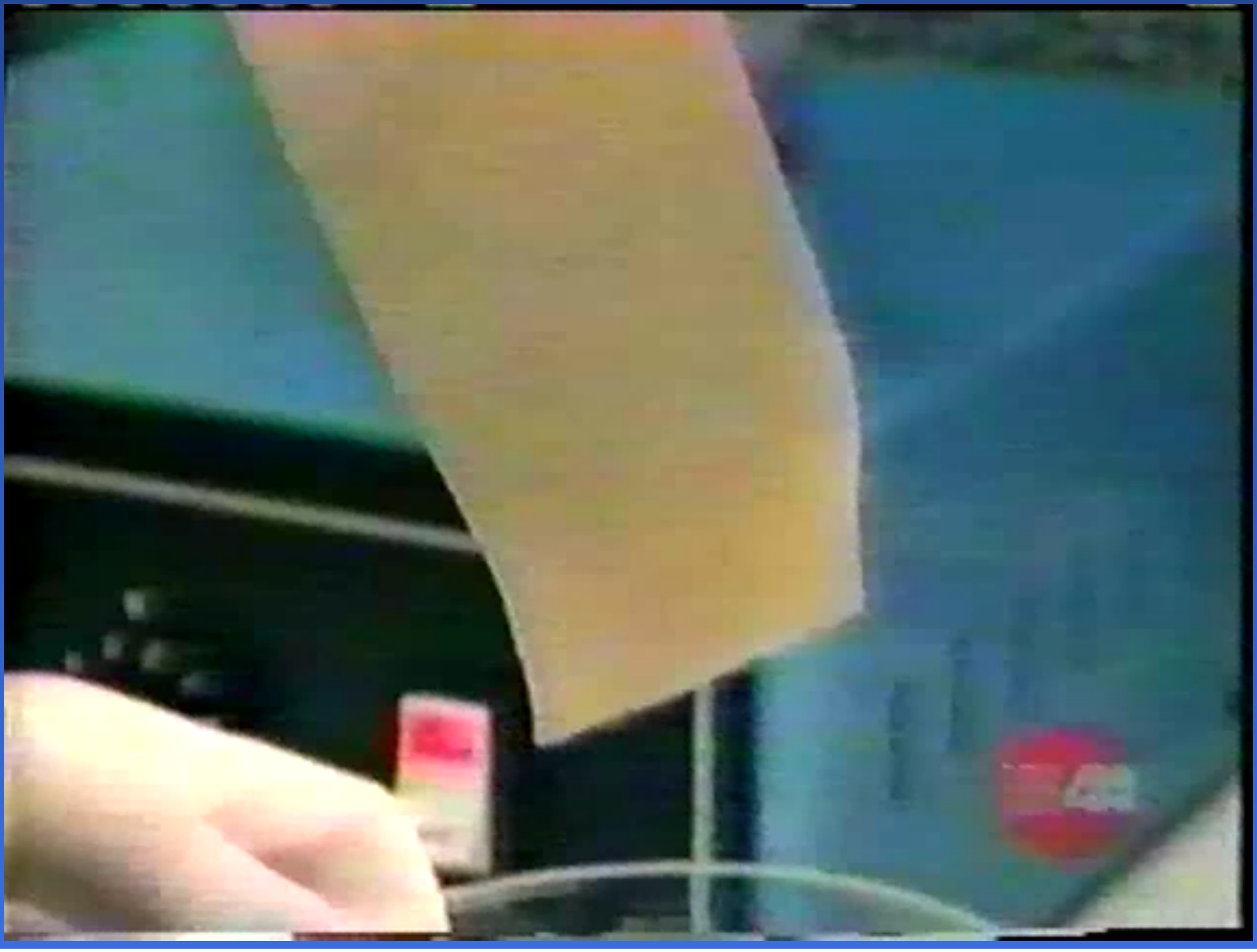
- Chemical Engineers have pioneered a new field of healthcare – which endeavors to repair or replace damaged tissue to an extent far beyond what naturally can occur.
    - Large sections of bone
    - Heart muscle damage
    - Loss of liver function
    - Burned Skin
    - Cartilage

Tissue Engineering

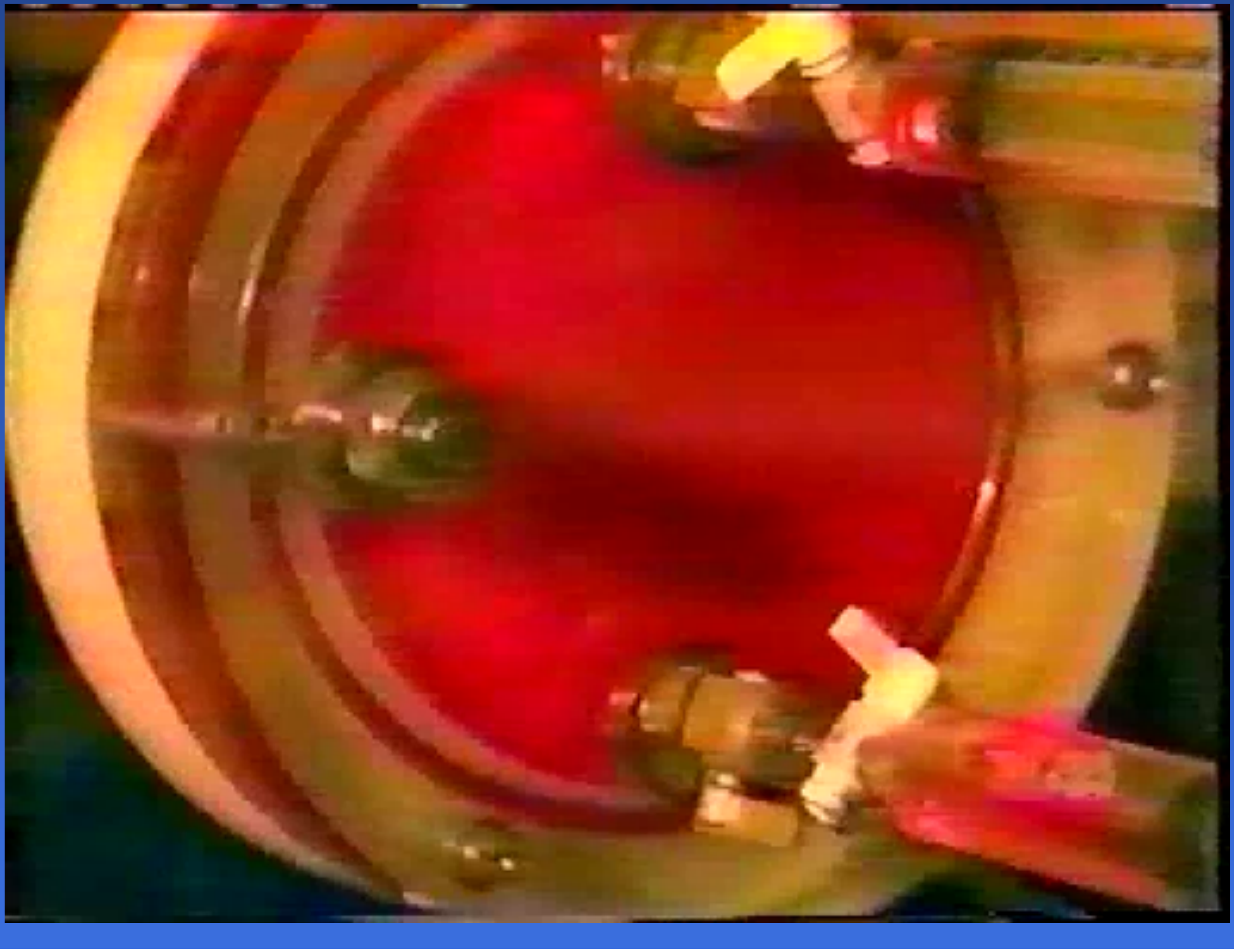
- This is more than just a biologist or MD problem because culturing and causing development of significant sections of tissue requires controlling the flow of nutrients to the material, the stresses that occur and the micro configuration so that the cells become the desired material
  - Essential challenge is vascularization

Synthesis of replacement parts for people

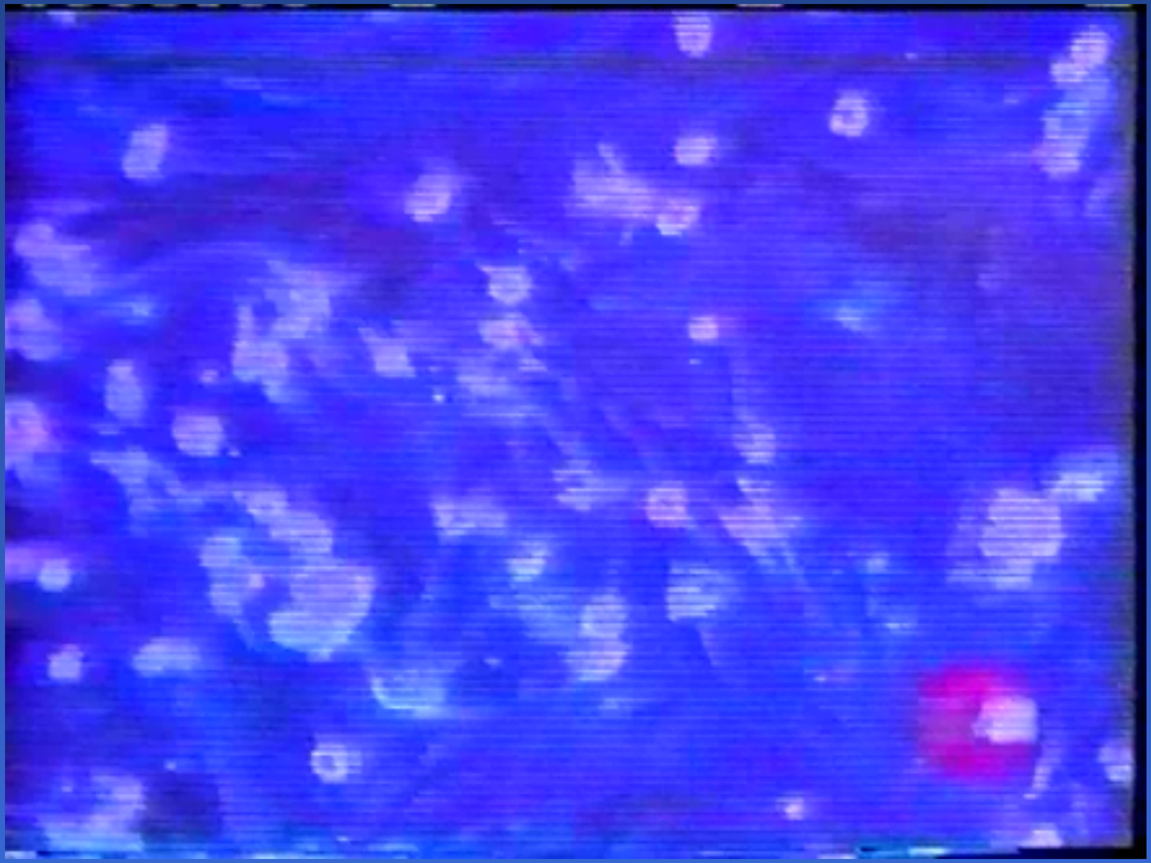
- **Bob Langer, Chemical Enginering Professor at MIT**
- **Alan Alda, One of Langer's students**
- **Video from *Scientific American Frontiers***



Chemical reactor for growing heart tissue



Synthetic heart cells



Liver “Chip”

- Tubes keep vitamins and nutrients pumping through the tiny "liver chip."

Transdermal glucose monitor

GlucoWatch G2 Biographer from Cygnus Inc.

Brain Cancer implantable “patch”

http://www.guilfordpharm.com/fs_products_f.htm

Also on the horizon

- New drug delivery technologies
  - Insulin pump: artificial pancreas
  - Other feedback control systems for drug administration
  - Addition of special ligands onto small molecule drugs to get them to bind at specific locations
  - Combined constructs of drug molecule and specially chosen particle size that help target delivery to specific locations (aerosols)

Connection with traditional chemical engineering

- The discipline is more than 100 years old.
- Chemical engineering originated with the need to bring to society products and molecules invented through chemistry.
- What is the connection between this and synthetic tissue or medical diagnostics?

The fundamental nature of our models allows broad application

Transport Phenomena and *Reaction Engineering*

Theoretical Analysis of Antibody Targeting of Tumor Spheroids: Importance of Dosage for Penetration, and Affinity for Retention[1]

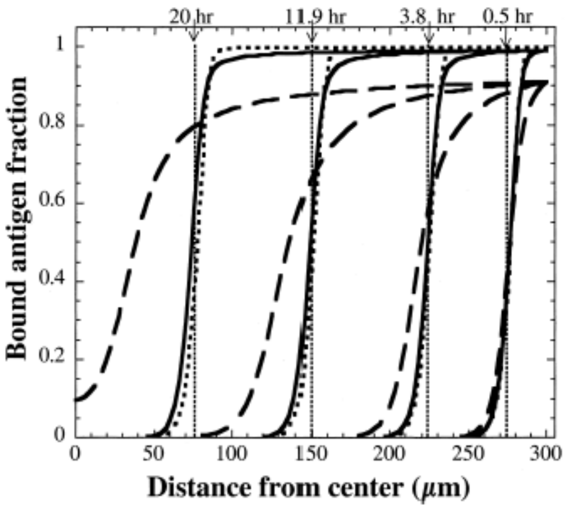
Christilyn P. Graff and K. Dane Wittrup[2]

The moving reaction front observed in these simulations is analogous to one described in the classic chemical reaction engineering literature. Combustion of carbon deposits in catalyst particles is observed to produce such moving fronts with outer shells and inner cores, and a simplified analytical theory termed the SCM[3] was derived to describe these phenomena (27, 28). The central assumption of the SCM is that diffusion from the surface of the sphere to the internal reaction front is significantly slower than consumption of the reactant at the reaction front at a critical radius r_c. The antibody spheroid

$$\frac{\partial Ab}{\partial t} = D\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial Ab}{\partial r}\right) - \frac{k_{on}}{\varepsilon}AbAg + k_{off}B$$

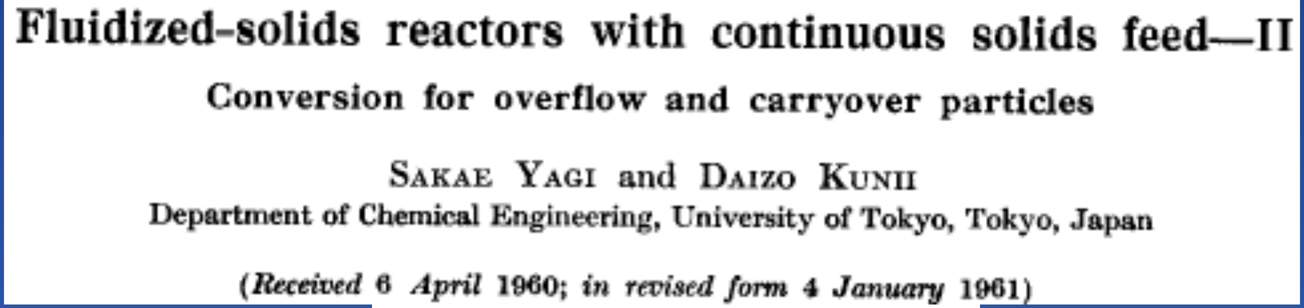
$$\frac{\partial B}{\partial t} = \frac{k_{on}}{\varepsilon}AbAg - k_{off}B - k_eB$$

$$\frac{\partial Ag}{\partial t} = R_s - \frac{k_{on}}{\varepsilon}AbAg + k_{off}B - k_eAg$$



From a paper in the journal "Cancer Research",2003 by two Chemical Engineers

Ideas for this analysis originated in about 1960



Fluidized-solids reactors with continuous solids feed—II

Conversion for overflow and carryover particles

Sakae Yagi and Daizo Kunii

Department of Chemical Engineering, University of Tokyo, Tokyo, Japan

(*Received* 6 *April* 1960; *in revised form* 4 *January* 1961)

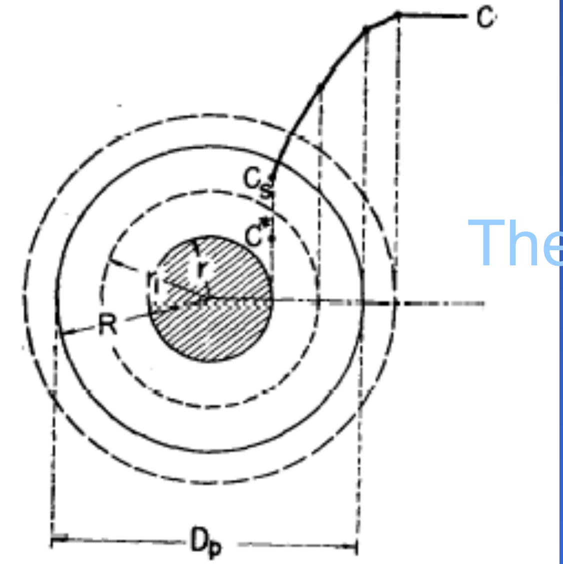
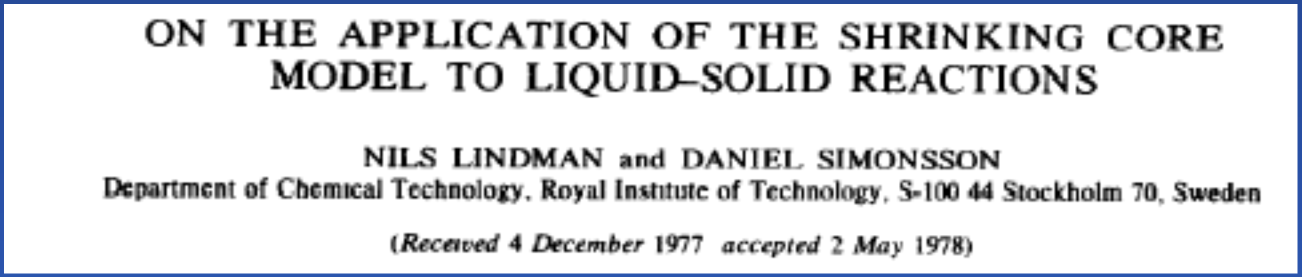


Fig. 1. Model of single particle, in which solid phase remains around the unreacted core. $D_p = x$.

The Shrinking Core!

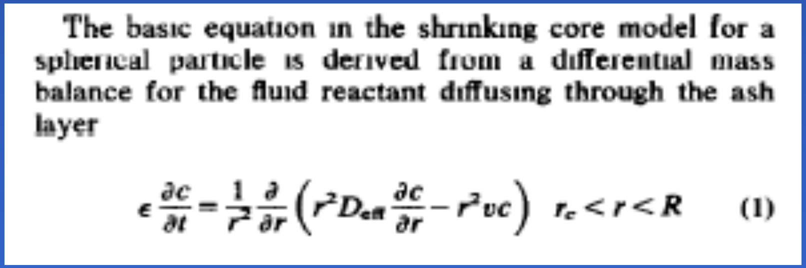
More mathematical analysis done in 1978



ON THE APPLICATION OF THE SHRINKING CORE MODEL TO LIQUID–SOLID REACTIONS

NILS LINDMAN and DANIEL SIMONSSON
Department of Chemical Technology, Royal Institute of Technology, S-100 44 Stockholm 70, Sweden

(*Received 4 December* 1977 *accepted 2 May* 1978)



The basic equation in the shrinking core model for a spherical particle is derived from a differential mass balance for the fluid reactant diffusing through the ash layer

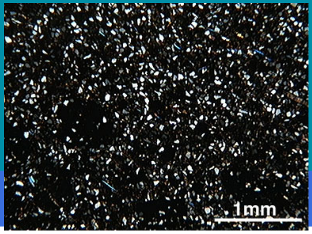
$$\epsilon \frac{\partial c}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_{\mathrm{eff}}\frac{\partial c}{\partial r} - r^2 v c\right) \quad r_c < r < R \qquad (1)$$

The fundamental nature of our models allows broad application

- Flow of oil in sandstone
  - Governing equation

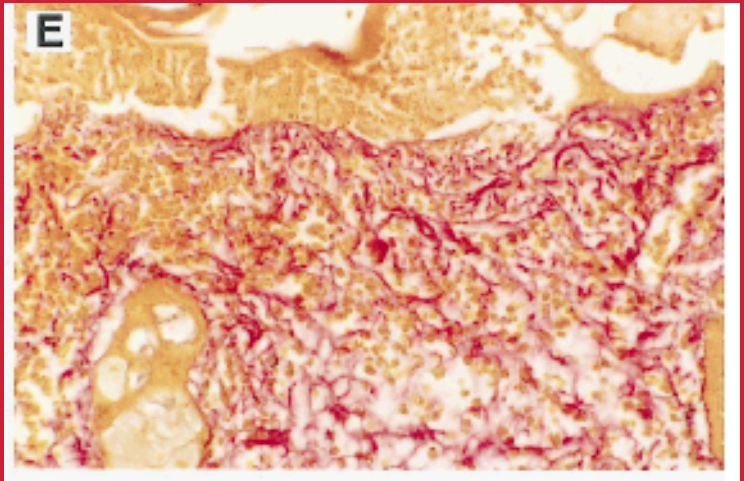
$$\frac{\partial P}{\partial t} - K_e \frac{\partial^2 P}{\partial x^2} = 0$$

  - P is the local pressure causing flow
  - K_e is an effective hydraulic “conductivity” the response of fluid flow to the change in pressure



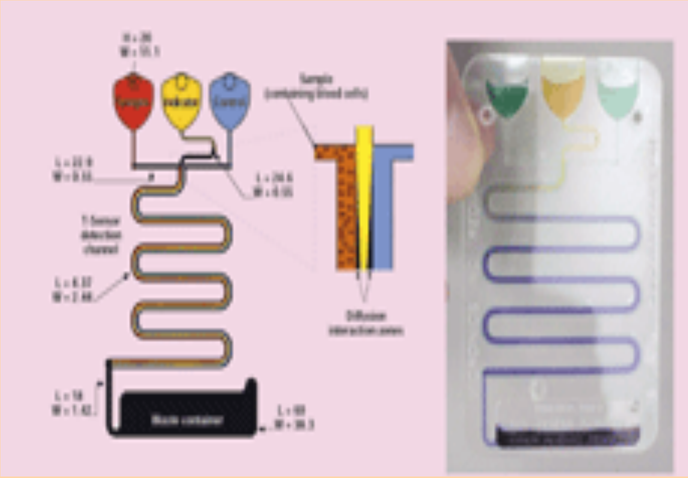
- Interstitial lymph fluid flow
  - Governing equation

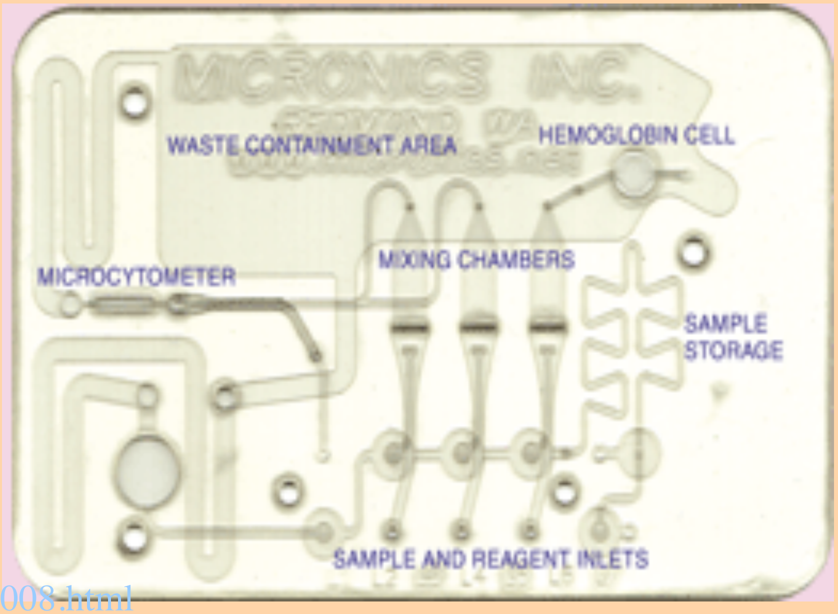
$$\frac{1}{(2\mu+\lambda)} \frac{\partial P^*}{\partial t} - K \frac{\partial^2 P^*}{\partial x^2} + \beta P^* = 0$$



Other applications of *Transport Phenomena*

- **Flow in microfluidic devices**
  - **When things shrink, qualitative differences occur.**
  - **For example, a miniature propeller would not pump fluid!**





http://www.devicelink.com/ivdt/archive/00/11/008.html

Comparing different engineering disciplines

- **A way to think of which kind of engineer you might want to be is to connect with your "inner self"**
  - **You know, ... from when you were 10 years old.**
    - **Or at least sometime before *education* changed who you are.**
  - **What about the world did you find most fascinating?**

Comparing different engineering disciplines

- *If:*
  - Mechanical engineering inherently deals with all of the mechanical devices of humankind.
- *If*
  - Civil engineering involves the design and construction of large structures.
- *If*
  - Electrical engineering deals with the materials and processes that allow communication systems and computers.
- *Then:*
  - Chemical engineering describes the processes of nature

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What do chemical engineers learn about to become one?

- Fundamental Science,
  - Mathematics, Chemistry, Physics, Biology

- Engineering science topics:
  - Chemical Thermodynamics
  - Transport Phenomena

- Integration of these in courses such as
  - Reaction Engineering, Separation Processes and Process Design

What do chemical engineers from Notre Dame do?

- Opportunities in *traditional* fields:
  - Petroleum and Chemical Industries
  - Graduate/Professional school
  - Food processing companies
  - Consumer product companies
  - Pharmaceutical companies
  - Electronic devices manufacturing

Opportunities in nontraditional fields

- Non-traditional fields that have an inherent chemical engineering component
  - see examples above
- Business analysis
  - Predicting oil/commodity prices
  - How much should Wal-Mart charge for DVD players ??
  - Financial analysis of new technologies
  - Investment Banking
  - Real Estate Pricing
- Political advising
  - A broadly-based science education is ideal for understanding important environmental issues that the world faces !!

First jobs of recent grads

- **Accenture (IT / business consulting)**
- **Bayer, Merck, Lilly (pharmaceuticals)**
- **Procter and Gamble (brand mgmt)**
- **UOP (process engineering)**
- **TRW (satellite systems)**
- **Merrill Lynch (investment banking)**
- **GE (aircraft engines division)**
- **Loyola (law school)**
- **Air Products (Career Development Program)**
- **I.U (medical school)**
- **Military (medical service corp, flight school)**
- **MIT, Stanford, UCSB, Minnesota (graduate school in chemical engineering)**
- **Eli Lilly (pharmaceuticals)**
- **BP, Marathon (Oil industry)**

Snapshot summary

- 10% business / consulting
- 25% professional / graduate school
- 25% chemical / petroleum industry
- 15% pharmaceutical industry
- 10% military
- 10% aerospace industry
- 5% marketing, financial services

Why can our graduates have such varied careers?

- Our program is broad and fundamental
  - Not geared toward a particular product or industry
- Traditional chemical industry is in stable phase
- Energy industry is in a rapid growth phase
- Pharmaceutical industry is evolving -- needs a new direction
- Other growth industries (IT, business consulting, financial services) recognize the value of a fundamental engineering education

Summary

- To summarize
  - The ability of chemical engineers to deal with chemical nature of materials from molecular to macroscopic length scales makes them unique.
  - These skills can be used in a number of areas outside of the chemical processing industries
  - The inherent breadth of the curriculum and our focus on understanding *why*, allows our graduates to make major impacts in a diverse range of fields where the ability to analyze problems quantitatively is important!