CHEMICAL ENGINEERING: PRESENT AND FUTURE

a topical survey

EMERGING AREAS

1. BIOENGINEERING

1.1. BIOPROCESS ENGINEERING

Bio-reactors
- analysis and design
- computer control
- continuous processing - beer, etc., produced in quantity

Large-scale tissue culture -
- plant and animal cells
- effect of mechanical shear, cell-surface interactions, materials for anchorage
- mass transfer/shear in large-scale tissue culture

Bioseparation and purification systems -
- super-critical fluid extraction
- membrane systems: osmosis/dialysis
- chromatographic characteristics
- electrophoresis

Monitoring and control
- biosensors -
  - CHEMFET - for chemical input
  - applications:
    - indwelling glucose sensors,
    - swallable sensors for GI tract
    - in-situ identification of tumors
    - field implanted sensors
    - on-line measurement
- spectroscopy -
  - MS, GC, LC, NMR for non-lab environment

Asepsis, containment and detection of trace contamination
- in large reactors

Risk assessment -
- releasing genetically altered micro-organisms into environment

Agriculture, food processing and waste treatment

Biosubstance database -
- enzymes, proteins, micro-organisms

Bioprocess applications of proteins
- environment-structure-function relations
- molecular recognition using antibodies
- biocatalysis
  - cofactor requirements and multiple enzyme catalytic sequence
  - enzymatic catalysis under abiotic conditions
- improved biocatalysts from protein engineering

Protein recovery
- equilibrium partitioning of protein mixtures
- interactions with interfaces
- affinity purification
- genetic engineering for enhanced separations

Protein processing -
- preservation, structure/bioactivity
- separation from dilute solutions

Catalytic and chemical functions of cells
- transport pathways, barriers, and facilitators
- activities in metabolic reaction networks
- regulation of metabolic network structure
- long-term genetic drift
- cell interactions with interfaces
- genetic engineering for chemicals production and degradation
- genetic engineering for broadly enhanced cell activity

Artificial enzyme templates -
- translation of chemical catalyst knowledge and simulation of catalyst, e.g., shape-selective zeolites, synthetic antibodies

Surface interactions - membrane transport

1.2. BIOMEDICINE

Historical perspectives
- hemodynamics
- water and solute transport
- pharmacokinetics in chemotherapy
- biomaterials
- organ analogs
- blood processing

Future directions
- interfacial phenomena in biological systems
  - liquid-solid interfacial phenomena
  - liquid-gas interfacial phenomena
- transport issues in biological systems
  - organ systems
  - intracellular systems
  - protein transport and dynamics
- macromolecular and cellular phenomena with an emphasis on recognition properties
  - protein science
  - cellular science

Protheses and biomaterials: medical devices
Medical diagnostics
Chemical synthesis of drugs
Computed-aided drug design
Genetic engineering and recombinant human proteins
Gene therapy
Drug delivery systems
Medical imaging
Angio-tension-converting enzyme inhibitors

Challenges to Chemical Engineers
- Human health
  - artificial organs, artificial tissues and prostheses
  - diagnostics
  - preventing and curing disease

Intellectual Frontiers
- Models for fundamental biological interactions
- Biological surfaces and interfaces
- Engineering analysis of complex biological systems

blood oxygenation by liquid membrane permeation
decompression sickness
thermal control in the human
oxygenators for infants
modeling respiratory control
flow and shear field in artificial heart valves
artificial kidney and its interaction with the host body

2. MATERIALS

2.1. POLYMERS, CERAMICS AND COMPOSITES

Synthesis of new polymeric materials
- polymers developing novel microstructures
  - block copolymers
  - liquid crystal polymers
  - polymerization in Langmuir-Blodgett films
  - silane and other non-carbon-backbone polymers
  - ion-containing polymers
- electrical, optical and magnetic properties of polymers
- biological synthesis of polymeric materials

Developments in polymer processing
- polymerization
- reactive processing
- processing of polymer composites

Emerging areas of polymer applications
- adhesion
- medicine
- electronics and photonics

Interdisciplinary character of polymer science
Theory: dynamics of polymers in bulk
New material development
- polymer blends
- biomaterials

Analytical techniques
- synchrotron SAXS
- Deuterium NMR
- SANS

Challenges to Chemical Engineers
- Polymers
- Polymer composites
- Advanced ceramics -- sol-gel processing
  chemical additives in ceramic processing
- Ceramic composites
- Composite liquids

Intellectual Frontiers
- Microscale structures and processes
  - new concepts in molecular design of composite materials
  - the role of interfaces in materials chemistry
  - understanding the molecular behavior of composite liquids
  - chemical dynamics and modeling of molecular processes

The intimate connection between materials synthesis and processing
processing of complex liquids
processing of powders
processing of polymers
process design and control
Fabrication and repair of materials systems
designing systems from the molecules on up
chemical processing in the fabrication of materials systems
detection and repair of flaws in materials systems
Plastic Components for Automobiles
Petrochemicals
Ceramics for Engines
Coating Technologies
Computed-aided Process Design
Food Packaging and Preservation
Materials for Housing
MATERIALS FOR THE FUTURE

2.2. MICROELECTRONIC AND OPTICAL MATERIALS

Electronic devices
Device fabrication
silicon production
lithography
Light wave media (optical fibers)
optical fiber manufacturing
thermophoresis
ultrapurifiction

Organometallic vapor phase epitaxy
experimental investigations
models
Plasma processing
experimental investigations
modeling approaches
Process control of microelectronics manufacturing

Current Chemical Manufacturing Processes
Microcircuits
Light wave media and devices
Recording media
Materials and devices for interconnection and packaging
Photovoltaics
Superconductors
Intellectual Frontiers
Process integration
Reactor engineering and design
Ultrapurification
Chemical synthesis and processing of polymeric materials
Chemical synthesis and processing of ceramic materials
Deposition of thin films
Modeling and the study of chemical dynamics
Engineering for environmental protection and process safety

Optical Fibers
Nanofabrication
Electronic Packaging
Optical Interconnection and Optoelectronic Devices
Display Technologies
Data Storage and Retrieval
Single-atom Manipulation
Microelectronics factory of the future

3. ENVIRONMENTAL PROTECTION AND ENERGY

Transport and transformation in the environment
Aerosols
- coal combustion aerosol formation
- aerosol and cloud chemistry
- nucleation
- chemical characterization of particles
- microcontamination control

Treatment of hazardous wastes
- incineration of hazardous wastes
- photocatalytic degradation of hazardous wastes on semiconductor surfaces

Energy-environmental interface
Photovoltaic power generation

Combustion chemistry
Reduction of combustion-generated pollution by combustion process modification
Char gasification reactions

Impact on society of chemicals in the environment
- chemical industry safety
- combustion of fuels for power generation and transportation
- hazardous waste management

Design of inherently safer and less polluting plants and processes
Combustion
- hydrocarbons and fuel-bound nitrogen
- soot
- ash
- sulfur oxides
- fires and explosions

Hazardous waste management
- detoxification of currently generated waste
  - thermal destruction
  - biodegradation
  - separation processes
  - wet oxidation
- remediation of toxic waste sites
  - separation processes
  - biodegradation
  - monitoring

Behavior of effluents in the environment

- the atmospheric environment
- the aquatic and soild environment
- ambient monitoring
- multimedia approach to integrated chemical management

Assessment and management of health, safety and environmental risks
- risk assessment
  - hazard identification and assessment
  - exposure assessment
- risk management

Technologies for exploiting energy resources
- enhanced oil recovery
- shale oil production
- conversion of coal to gaseous and liquid fuels
- new raw materials for petroleum refineries
- municipal solid waste as an energy source
- nuclear energy
  - nuclear fission
  - nuclear fusion
- electrochemical energy conversion and storage
- solar power
- geothermal energy
- plant biomass as a fuel source

Technologies for exploiting mineral and metal resources
- high-concentration raw materials
- low-concentration raw materials
- waste streams as sources of minerals and metals

Intellectual frontiers
- in-situ processing
- processing solids
- separation processes
- materials
- advanced methods for design and scale-up
- other important research

Designer gasoline
Liquid fuels from natural gas, coal and shale
Fuel-efficient and low-emission vehicles
Portable electric power
Fuel cells
Nuclear energy: promise and problems
Solar-electric power generation
Solar-photoelectrochemical cells
Catalytic cracking

Atmospheric chemistry
Life cycle analysis
Risk and impact analysis
Manufacturing with mineral environmental impact
Control of power plant emissions
Environmentally friendly products
Recycling
Separation and conversion for waste reduction
Cleaning up contaminated sites
Catalysts for control of automobile exhaust

SUBDISCIPLINES

1. FLUID MECHANICS AND TRANSPORT PHENOMENA

The future - challenges and opportunities in research
- nonlinear systems
- computational simulation
- fluids with microstructure

Directions for the future
Examples from the present
- single crystal growth from the melt
- mixing in deterministic flows
- flow of granular materials
- optical characterization of complex fluids
- finite element solutions of free surface flows
- simulations of the dynamics of dense dispersions

Nonlinear dynamics - examples:
- polymer melt processing
- two-phase flow in porous media
- heat and mass transfer in pipe flow

2. THERMODYNAMICS

Modern methods
- macroscopic correlation methods
- molecular theory
- computer simulation
- computer graphics
- intermolecular potentials

Current problems
- phase equilibria of complex systems
- fluid behavior in micropores

The future
- research
  - computer-aided materials design
  - surface phenomena
  - biotechnology and biomedicine
  - phase equilibria and fluid properties

Semiempirical correlations for conventional processes
Thermodynamics for rate processes, including catalysis
Integration of thermodynamics into the broad concerns of chemical engineering

Microstructural fluids: a primer
Microstructural fluids: theory and simulation

3. KINETICS, CATALYSIS AND REACTOR ENGINEERING

contemporary challenges
- representation of rate and equilibrium processes
- reactor modeling
- catalysis

Chemical reactor modeling
Kinetic modeling
Integration

Catalytic Design -
- The catalytic design problem
- Catalytic surfaces
- Transport within pores
- Catalytic impregnation profiles
- Catalyst particle shape
- An industrial example

Chemical Transport Reactions -
- microlithographic processes
- electron-beam lithography polymers
- resists for pattern-transfer
- plasma etching
- coating and dissolution processes
- dissolution rate measurements using laser interferometry

expt./theor. study of CVD processes
laser diagnostics of silicon CVD
low pressure CVD of silicon nitride
modeling low pressure CVD reactors
reactor analysis of Si deposition by CVD using disilane

metal organic CVD at stagnation point
spectroscopy of organometallic CVD
kinetics of tungsten CVD
decomposition kinetics of hydrides in CVD of III-V semiconductors
design considerations/alternatives for epitaxial CVD reactors
reactor design for growing compound semiconductor epitaxial layers

CVD in a Siemens decomposer
silane pyrolysis: nucleation control
modeling semi-conductor film growth
modeling of glow discharge reactors
theor./expt. study of parallel-plate plasma etching
kinetic analysis of polysilicon etching in discharges
rf-discharge plasma etch chemistry

4. PROCESS ENGINEERING

Design in process engineering - a model of the design process
Synthesis - Expert Systems
Analysis
- steady-state modeling
  - flowsheeting programs
  - convergence
- dynamics
  - stiff equation sets
  - the index problem
  - architectures for simulators
- partial differential equations
- optimization

Process Control Theory -
- The role of process control theory and experiment
- Control theory of the 1960s and 1970s
- Model predictive control
- Robust process control
- Control structure selection
- Some research topics for the next decade

- A hierarchy of paradigms
- A process engineering paradigm
  - hierarchies of designs
  - a higher-level process understanding
  - "high value added" products
  - conceptual design of batch versus continuous processes
  - new computer aided design tools
- A hierarchical approach to conceptual design
  - products, by-products and recycles
  - separation system specification
  - heat exchanger networks
  - control system synthesis and safety

Symbolic Computing and Artifical Intelligence in Chemical Engineering:
- Computing in chemical engineering
  - process design
  - product and process development
  - understanding system behavior
  - feedback control
  - monitoring and diagnosis of process operations
  - planning and scheduling of process operations
- The essential framework of artificial intelligence applications in chemical engineering
  - making a mind versus modeling the brain
  - AI and computer programming
  - modeling knowledge
  - problem-solving paradigms
- Descriptive simulation of physiochemical systems
- Formal description and analysis of process trends
- Planning of process operations
- Conceptual design of chemical processes

- Computer-assisted process and control engineering -
  - Mathematical Models of Fundamental Phenomena
    - Hydrodynamic systems
    - Polymer processing
    - Petroleum processing
      - combustion systems
      - environmental systems
  - Process Design
    - Computer-aided design of new processes
    - Computer-assisted process retrofitting
    - Research opportunities in process design
  - Process Operation and Control
    - Measurement
    - Interpretation of process information
    - Integration of process design with control
    - Robust and adaptive control
    - Batch process engineering
  - Process Sensors
    - Future sensor developments
    - Research opportunities
  - Process Engineering Information Management
  - Implications of Research Frontiers

5. SURFACES, INTERFACES AND MICROSTRUCTURES

- The nature of structure
- Relationship to applications of chemical engineering
- Biochemical and biomedical engineering
- Electronic, photonic and recording materials and devices
- Polymers, ceramics and composites
- Processing energy and natural resources
- Environmental protection, process safety and hazardous waste management
- Intellectual Frontiers
  - Catalysis
    - catalyst synthesis
    - characterization of catalyst structure
    - surface chemistry
    - catalyst design
  - Electrochemistry and corrosion
    - charge transfer
    - molecular dynamics
    - supramolecular microstructures
  - Electronic, photonic and recording materials and devices
    - characterization of microstructure
    - photoresist processing
    - chemical vapor deposition and plasma deposition/etching of thin films
    - mathematical modeling
  - Colloids, surfactants and fluid interfaces
  - Ceramics, cements and stuctural composites
  - Membranes
- Research Needs
  - Instrumentation

microscopy and microtomography
scattering methods
resonance spectroscopies
other important methods
cost and availability

Theory

6. PARTICLE SCIENCE AND TECHNOLOGY (PARTICUOLOGY)

Basic Problems in Particle Science and Technology -

- Particle measurement, mathematics
- Particle measurement, techniques
- Sampling
- Particle mechanics
- Physics of particulate solids
- Flow of fluid through particulate media
- Multi-phase flow of particulate systems

Applications -

Metallurgy	iron and steel from powdered solids
Petroleum prod.	tertiary oil recovery; drilling mud
Petroleum ref.	particle size design for FCC catalyst
Chemical	particle size control for titanox
Environment	mechanism of fog formation
Defence	filtration of radioactive particles
Power	high-temp. dust removal for turbines
Coal	improved combustion for FBC
Nuclear	reprocessing of reactor fuel
Mining	control of coal dust explosion
Transportation	icing of aircraft propellers
Medicine	passage of particles through membranes
Pharmacy	tableting, pelleting, mixing
Building	exfoliation of pearlite
Agriculture	grain drying and transportation
Food	milk powder, minute rice

particle characterization -- size, shape, etc.
sampling and sample preparation
particle generation, preparation, pre- and after-treatment
separation -- S/S, S/G, S/L; filtration
aerosol
slurry
size reduction -- crushing, grinding and comminution
agglomeration
conveying - bulk, pneumatic, hydraulic
storage
solids feeding and metering
flocculation
chemical reaction
fluidization
health and safety
magnetic/electrostatic effects
instrumentation and measurement
microscopy