# Vision 2020:
# Reaction Engineering Roadmap

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# FOREWORD

The *Reaction Engineering Roadmap* is a part of an industry-wide effort to create a blueprint of the research and technology milestones that are necessary to achieve long-term industry goals. This report documents the results of a workshop focused on the research needs, technology barriers, and priorities of the chemical industry as they relate to reaction engineering viewed first by industrial use (basic chemicals; specialty chemicals; pharmaceuticals; and polymers) and then by technology segment (reactor system selection, design, and scale-up; chemical mechanism development and property estimation; dealing with catalysis; and new, nonstandard reactor types). The workshop brought together forty-six experts from the chemical industry, its customer industries, universities, and government research laboratories. The workshop was a part of the chemical industry's effort to develop its technology roadmap for the future.

This document must be viewed as evolutionary in nature. While the *Reaction Engineering Roadmap* presents an impressive compilation of critical chemical industry research needs, the workshop was necessarily limited in time, scope, and participation, and the emerging roadmap may not fully incorporate all needs. Every effort was made to include a broad range of industry participants, but it is inevitable that valuable ideas may have been left out. Thus, this document should be considered a work in progress to develop consensus on industry research needs. It will evolve as additional information becomes available. It is also closely linked to other technology roadmaps developed to support the chemical industry: new process chemistry, biotechnology, materials, separations, and computational technologies. These roadmaps can be obtained at www.chemicalvision2020.org.

# I. SUMMARY

**Background:** The Reaction Engineering Roadmap has been prepared based on the information gathered in a workshop held in conjunction with the 1999 Annual American Institute of Chemical Engineer's meeting in Dallas, Texas on October 30–31, 1999. The workshop brought together forty-six experts from the chemical industry, its customer industries, universities, and government research laboratories to brainstorm on research needs for reaction engineering. The workshop was held to develop a path to overcome the barriers and challenges identified in *Technology Vision 2020: The Chemical Industry*. *Technology Vision 2020* details the challenges faced by the U.S. chemical industry as it strives to maintain its competitive position into the next millennium. The details of the workshop, including technical presentations, are given in the appendices.

Workshop participants were asked to define the present challenges faced by industries producing and using chemicals and to identify the technical barriers and the research needs required to overcome those barriers. The participants identified research that will be important in contributing to a 30% reduction in relative indicators for material usage, water consumption, toxics dispersion, and pollutants dispersion by the year 2020 for the chemical industry. The relative indicators are those being tested by the National Roundtable for the Environment and the Economy where material usage, for example, is indexed to the selling price of the product minus the cost of raw materials.

**Roadmap Results:** A small number of research areas were identified as key focus areas that will provide the foundation for improvements in reaction engineering: experimental tools and online sensors, fundamentals-based modeling, thermodynamic and transport property data, and system integration. Improved experimental tools and sensors are needed to provide input data for models. Improved models are needed to design reactors effectively and to optimize the process chemistry. Thermodynamic and kinetic data are needed as input into these models. System integration is needed to provide user-friendly results and accomplish the tasks in a cost effective, timely manner. The resulting information will be used to support research in reactor design and scale-up, chemical mechanisms, catalysts, and new reactor development. The research identified in Tables I.1 and I.2 should result in optimized, integrated reactor systems with higher product selectivity, yield, and purity. They should consume less raw material, use less energy and water, generate less waste, and be more easily adapted to the production of new products. The systems integration approach to development and plant operations should reduce the time and costs associated with implementing new technologies and bringing new products to market.

**Research Needs:** The workshop participants formulated research needs by industrial and by technology segments. The resulting research needs were prioritized and sorted by time frame. The *highest priority* key research needs that were identified are summarized below:

*Basic Chemicals:* Develop more efficient methods to build process models, obtain and predict physical, chemical, and transport property data and to verify model results.

*Specialty Chemicals:* Develop models to predict product properties *a priori,* to facilitate reactor/process selection and design, and to increase reaction selectivity. Develop reactor design that can be adapted more easily to multiproduct manufacture.

*Pharmaceuticals:* Develop better experimental screening techniques to reduce development time and costs, use combinatorial techniques to evaluate synthesis routes, thermochemical and thermophysical properties data for complex systems, more selective catalysts, and improved reactor design for high purity/selectivity/yield.

*Polymers:* Develop the ability to link process conditions to product properties (at the micro-, meso-, and macro-scales), develop better fluid dynamics models that account for interaction effects of large complex molecules, and create process monitors that can track polymerization progress on line.

*Reactor System Design and Scale-up:* Establish better procedures for characterizing the operation of lab, pilot and plant reactors and cross correlating their behavior. Develop more efficient methods to obtain physical, chemical, and transport property data for input into and verification of models.

*Chemical Mechanisms:* Develop micro-kinetic experimental capabilities, methods to integrate solvent effects into reaction models, tools to couple process chemistry and process modeling, and methods to determine macroscopic properties and kinetic behavior from molecular structures.

*Catalysis:* Develop better in situ characterization and sensing tools, system integration techniques to optimize catalyst and reactor operations simultaneously, catalysts for solid matrices, and fuel cell focused catalysts.

*Novel Reactors*: Development of nonstandard reactors is dependent on advances in fundamental research and enabling technologies. Research areas include intensified reactors, rapid heating and cooling techniques, structured contacting, external field-assisted and photochemical reactions, and reactors for extreme conditions. Enabling technologies include new materials development, systems integration, micro-scale properties and phenomena determination, multistage design capabilities, and self-assembling reactor development.

**Cross-Cutting Research Needs:** Major research needs that cut across several or all of the technical areas were identified. These fell into four technical categories: experimental tools, modeling and property estimation, sensors, and system integration. Improved experimental tools are needed to design and operate reaction engineering systems more efficiently and to provide input data for models. These include better designs for laboratory-scale reactors and better experimental techniques for screening of synthesis methods and for developing a fundamental understanding of plant system operations. Fundamentals-based models are needed to support design and operation of reaction engineering systems. Thermophysical, thermochemical, and transport data that describe complex systems are needed for input into and validation of these models. Fast, precise, robust, online sensors are needed for data collection, monitoring, and process control. Integration of all these research capabilities into a systems approach is required to develop viable production reactors for industry. There is a need for better integration of models and experimental data gathering as well as models which couple process chemistry with process modeling. Ultimately, design and optimization tools are needed which will link process conditions to product properties at the micro-, meso-, and macro-scales.

**Key R&D Linkages:** Tables I.1 and I.2 show the linkages between key research needs and the time frame for obtaining the research results. Table I.1 summarizes the more general cross-cutting research areas, while Table I.2 addresses specific research needs for the major technical areas associated with reaction engineering. The linkages indicate where the results from one or more research areas provide important support to other areas either in the same or another time frame.

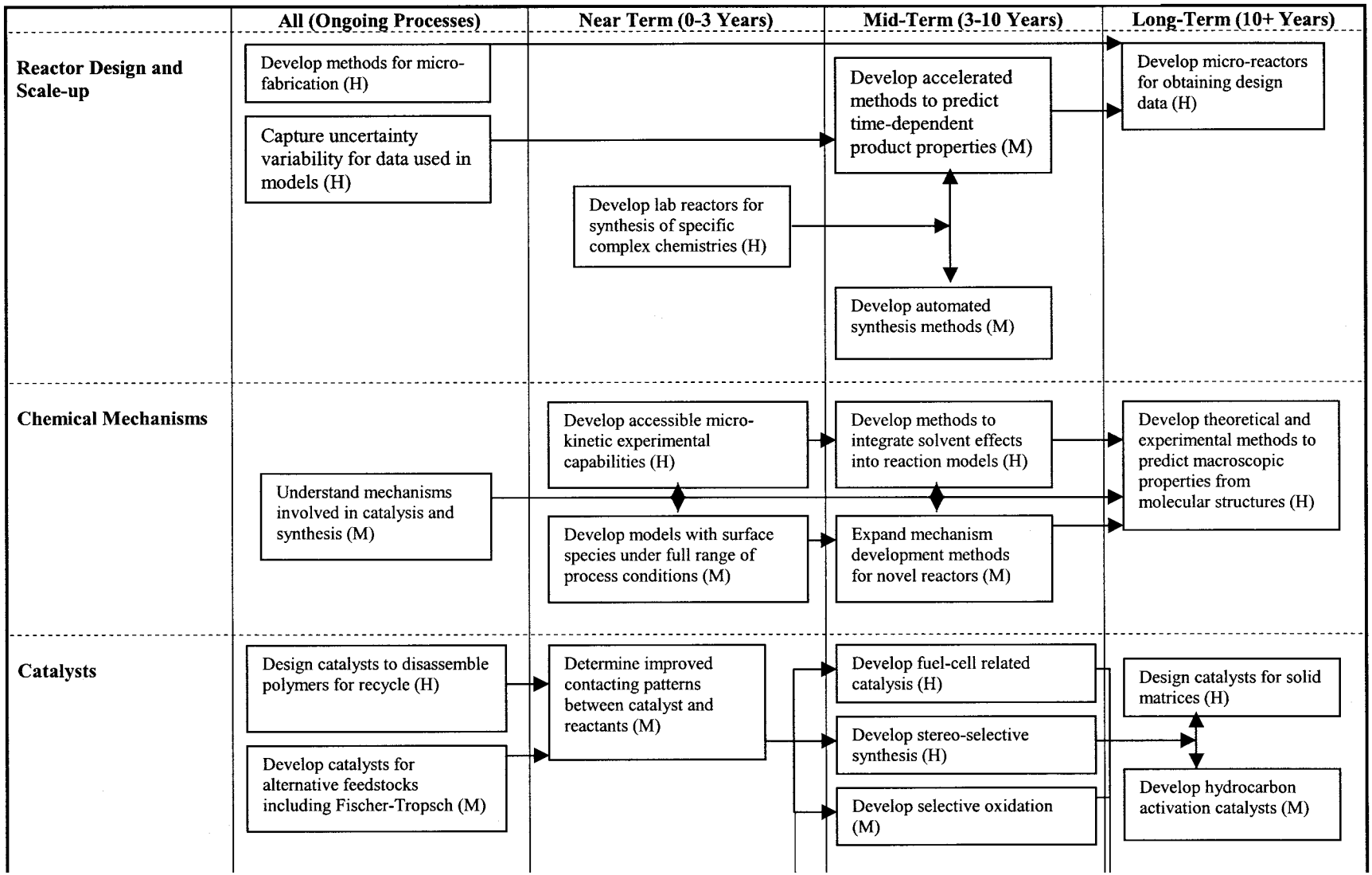
Table I.1 summarizes the major research needs for the four cross-cutting areas: experimental tools, modeling and property estimation, sensors, and system integration. Tasks in the cross-cutting technical areas are needed to support all aspects of future reaction engineering research. Improved experimental tools and sensors are needed to provide the data for models and system integration. Improved models are needed to design new reactors and make major chemistry changes. System integration is needed to accomplish this in a cost-effective, timely manner. The results from all four cross-cutting areas will support research in reactor design and scale-up, chemical mechanisms, catalysts, and new reactor development. Table I.2 summarizes key research linkages within each of these specific technical areas.

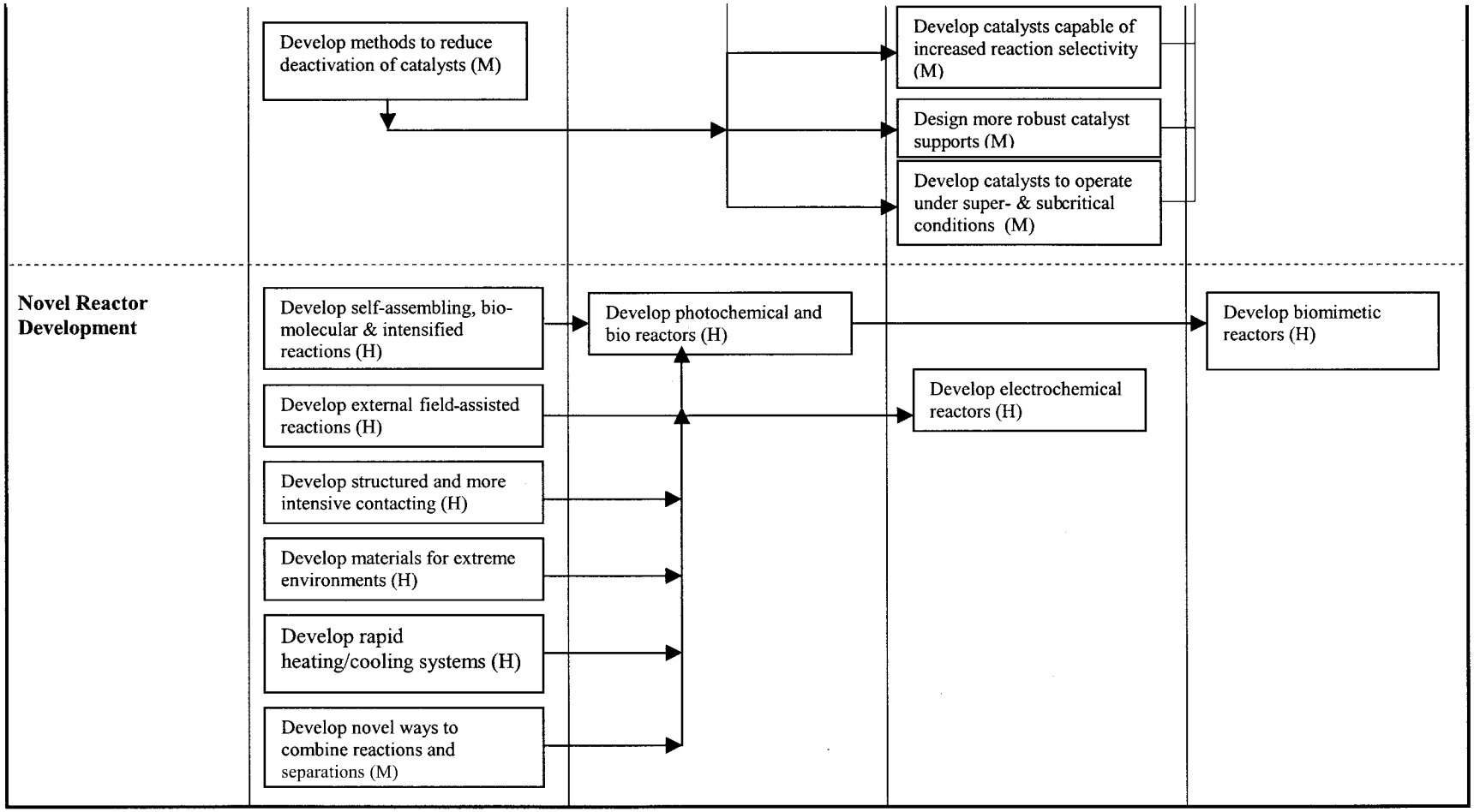
**Research-Related Needs:** Several research-related needs were also identified. These are needs/issues that are not truly research but are closely related. They include institutional, regulatory, and educational issues. The major research-related needs identified included (a) increase interdisciplinary education at universities, and (b) reduce the time and cost for bringing new processes on line and new products to market.

**Table I.1 Key R & D Linkages for Cross-Cutting Areas in Reaction Engineering**
(H = High Priority, M = Medium Priority)

| | All (Ongoing Processes) | Near Term (0-3 Years) | Mid-Term (3-10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| **Experimental Tools** | Development better screening techniques (M) | Improve characterization for lab-scale reactors (H) | Improve laboratory reactor designs (H) | Develop fundamental understanding of plant-scale processes (M) |
| **Modeling** | Obtain thermophysical, thermochemical, and transport data for input & validation of models (H)<br>Obtain data for model validation across multiple scales (H) | Develop models of reactions with mixing and transport (H)<br>Develop reactor synthesis models (H) | Develop CFD models with catalysts, multiple large molecules, & multi-phases (M) | Develop fundamentals-based models for catalysis design, synthesis chemistry, and reactors (M) |
| **Sensors & Controls** | | Develop on-line sensors (M) | Develop smart sensors (M) | |
| **System Integration** | Develop system optimization & design tools which link process conditions to product properties at all scales (micro, meso, and macro) (H) | | Combine experimental and modeling tools for kinetics and reactor design (M) | Develop practical tools which couple process chemistry with process modeling (H)<br>System integration to optimize catalyst and reactor at the same time (H) |

**Table I.2 Key R & D Linkages for Major Technical Areas in Reaction Engineering**
(H = High Priority, M = Medium Priority)




Develop methods to reduce deactivation of catalysts (M)
Develop catalysts capable of increased reaction selectivity (M)
Design more robust catalyst supports (M)
Develop catalysts to operate under super- & subcritical conditions (M)
Novel Reactor Development
Develop self-assembling, bio-molecular & intensified reactions (H)
Develop photochemical and bio reactors (H)
Develop biomimetic reactors (H)
Develop external field-assisted reactions (H)
Develop electrochemical reactors (H)
Develop structured and more intensive contacting (H)
Develop materials for extreme environments (H)
Develop rapid heating/cooling systems (H)
Develop novel ways to combine reactions and separations (M)

# II. INTRODUCTION

**Background:** Several years ago, the U.S. Department of Energy/Office of Industrial Technologies (DOE/OIT) identified several industries that have major roles in either raw materials production and/or consumption, energy usage, and waste generation. Prominent among them was the chemical industry. DOE/OIT is working with these industries to develop vision documents defining goals for the Year 2020 related to reduced raw material and energy usage and lowered waste generation. Goals have been developed for the chemical industry in a cooperative effort among DOE/OIT, the American Chemical Society, and the American Institute of Chemical Engineers, the Synthetic Organic Chemical Manufacturers Association, and the Council for Chemical Research. These goals and action proposals are detailed in the publication entitled *Technology Vision 2020: The Chemical Industry*.

DOE/OIT has further encouraged the individual industries to prepare technology roadmaps that will lead to meeting their respective Vision 2020 performance targets. A technology roadmap is analogous to an automobile roadmap employed in traveling from Point A to Point B. In the case of driving, the driver knows where he is (Point A), where he is going (Point B), and he has some knowledge of the terrain between points (A) and (B). In the case of a technology roadmap, the current state of the technology (A) and the desired future state (B) are defined. Then, the barriers to the journey and an identification of the possible research routes available to complete the journey are identified and prioritized.

**Trends and Drivers:** Factors that will influence industry in 2020 include: fossil fuel availability and prices; environmental regulations; growth in alternative processing technologies, such as biotechnology; recycling; use of total life cycle evaluations in decision-making processes; information technology; international competition; and the industrial growth rates in Asia, Europe, and North America. Several key factors will drive the need to change industrial practices. The public is expected to demand increases in pollution prevention/reduction and public safety, the value of fresh water will increase significantly, the cost for raw materials will increase, and improved access to and availability of information will change the industry. To remain competitive in the future, the chemical industry will need to tighten product specifications, reduce investment and operating costs per unit output, and increase the flexibility of plant operations.

At the present time, polymers and commodity chemicals (and their intermediates) represent the dominant market for innovation and growth. However, today's major chemical companies are increasingly pursuing a strategy based on tailoring specific products to target markets. Thus, materials, specialty chemicals, pharmaceuticals, performance polymers and some high-value petrochemicals represent the dominant future growth markets. Changes will be required to address increases in production volume and waste generation. Use of alternative fuels, such as natural gas and biological feedstocks, is also likely to increase.

Since the chemical reactor is the heart of any chemical process, reaction engineering will play a major part in maintaining industrial competitiveness. The potential for greenhouse gas reduction and pollution abatement will come from redesigning chemical reactors to produce less undesirable byproducts. Chemical reactors are likely to become smaller and more flexible. New technology is likely to integrate chemical reactions, transport phenomena, and separations processes into single unit operations. Modeling and simulation will reduce process development time as they provide a sharper focus on the key developmental problems that need to be solved and guide experimentation accordingly.

**Goals:** The general goal for the road-mapping workshop was to identify research needed to meet the chemical industry's vision. Elements of that vision include: maintaining or achieving positions of a leader in technology development; enhancing the quality of life; providing excellence in environment, safety, and health; good community relationships; seamless partnerships with academia and government; and promoting sustainable development.

The specific goals of the reaction engineering workshop were: (a) to define critical technology developments in reaction engineering needed to sustain the competitiveness of the U.S. chemical industry, (b) to identify trends and drivers that will dictate the timing and priority of the above technology developments, (c) to link these needs to the achievement of sustainability goals established for other roadmaps supporting Vision 2020, and (d) to define

the barriers to achieving the needed developments and means for overcoming them.

Visions and related roadmaps require commonly understood and communicated goals. By their nature, goals require some sort of indicator or yardstick. A group of companies working with the National Roundtable for the Environment and the Economy (NRTEE) developed indicators for material, energy, mass of pollutants, and water usage relative to the difference between the selling price of products and the cost of their raw materials. The NRTEE indicators are shown in Table II.1. For roadmapping purposes a target has been proposed for the chemical industry of 30% reduction in all five of the indicators shown in Table II.1 by the year 2020.

**Reaction Engineering Workshop:** The workshop was held in Dallas on October 30–31, 1999, and was attended by forty-six representatives from industry, academia, and the government. Full details of these meetings are provided in Appendix A. Participants in the workshop are shown in Appendix B.

Breakout sessions were used in each workshop to allow participants to focus on their technical area of expertise. Each breakout group was asked to scope out the technical challenges facing reaction engineering in order for it to be used to meet the workshop yardstick goals, identify technical barriers to meeting those challenges, and to list and prioritize the research needed to address the barriers. The workshop participants were initially asked to identify reaction engineering technical barriers and research needs within the industries with which they were most familiar, including basic chemicals, specialty chemicals, pharmaceuticals, and polymers. These industry needs were then used as the basis for identifying what research was needed in each of four key reaction engineering technical development areas: reactor design, chemical mechanisms, catalysis, and novel reactors. Participants sorted the latter prioritized research needs into four broad time frames in which they should be conducted: 0–3 years, 3–10 years, 10+ years, and ongoing. The results are summarized in Sections III – IV of this report. The detailed technical barriers and research needs identified in the breakout sessions are given in Appendix C. Major chemical industry statistics and presentations given at the workshop to set the stage for the brainstorming sessions are given in Appendices D and E, respectively.

**Roadmapping:** A smaller working group of people who attended the workshops used the output of the break out sessions to develop the roadmap given in this document and refine the linkages between the R&D needs. Linkages are important to identify because they identify instances of synergy between research activities that can be exploited to accelerate progress toward the roadmapping goals or reduce the cost of the research required. Several industrial workshop participants reviewed the results to assure accuracy of the final product, which is given in Section I.

**TABLE II.1**
**National Roundtable for the Environment and the Economy Indicators**

| | |
|---|---|
| *Material Indicator* | $MI = \dfrac{Mass\ of\ material\ purchased\ (MT) - Mass\ of\ product\ (MT)}{Revenue\ (US\$) - Cost\ of\ purchased\ materials\ (US\$)}$ |
| *Water Consumption Indicator* | $WCI = \dfrac{Volume\ of\ fresh\ water\ used^{a}\ (m^3)}{Revenue\ (US\$) - Cost\ of\ purchased\ materials\ (US\$)}$ |
| *Energy Indicator* | $EI = \dfrac{Net\ energy\ used\ (fence\ line)\ (MJ)}{Revenue\ (US\$) - Cost\ of\ purchased\ materials\ (US\$)}$ |
| *Toxics Dispersion Indicator* | $TDI = \dfrac{Total\ mass\ of\ recognized\ toxic\ materials\ released^{b}\ (MT)}{Revenue\ (US\$) - Cost\ of\ purchased\ materials\ (US\$)}$ |
| *Pollutants Dispersion Indicator* | $PDI = \dfrac{Total\ mass\ of\ recognized\ pollutants\ released^{c}\ (MT)}{Revenue\ (US\$) - Cost\ of\ purchased\ materials\ (US\$)}$ |

[a] Definitions are required (e.g., non-contact cooling water, etc.).

[b] Using a nation's most recognized list (the Toxic Release Inventory in USA, National Pollutant Release Inventory in Canada, etc.)

[c] The Pollutant Dispersion Indicator would include greenhouse gases, acid rain gases, eutrophication materials, ozone depleting chemicals, etc.

# III. INDUSTRIAL SEGMENTS RESEARCH NEEDS

## III.A. Basic Chemicals

**Summary:** Technical experts in reaction engineering identified the top research priorities for the basic chemicals industry to be (a) develop the ability to predict physical/chemical and transport property data, and (b) improve methodology for experimentally verifying computational models. The key research needs are listed in Table III.A.1, while the complete list of prioritized barriers and research are provided in Tables C.A.1 and C.A.2 in Appendix C.

**Situational Analysis:** The current chemical reactor technology in the basic chemicals industry is mature. Equipment is basically the same as it was twenty years ago. Existing reactors work well, but analysis of their operation does not provide the complete understanding required to optimize an existing process or apply the technology to a similar process. A major reason for this lack of understanding is that heat and mass transport are not well characterized.

The limitations associated with current reactors are due to (a) lack of confidence in using existing tools in reactor design, such as property/correlation techniques, (b) new advanced theory based tools are still in an early stage of development, and (c) there are not reliable approaches for validating these tools under realistic operating conditions. As a result, full-blown pilot plants are still required for process scale-up. Safety is predominant, often preventing operation at conditions that would be optimal for plant-scale performance. Materials available for reactor construction often constrain economic optimization.

Innovations in the industry have recently been driven by regulations, especially those related to the production of clean fuels and their combustion. Because of the limitations described above, these innovations have been achieved by old-fashioned "brute force" empirical methods, rather than by approaches based on a more fundamental understanding of the basic chemistry and physics of the processes.

In 2020, energy for the manufacture of chemicals will come from a variety of sources, with near zero emissions of gases other than pure $H_2O$ and clean $CO_2$. Even clean $CO_2$ emissions will be controlled. Part of the $CO_2$ will be

**Table III.A.1**
**Key Research Needs for Basic Chemicals**
(H = High Priority, M = Medium Priority)

| **Fundamental Science and Data *(H)*** | **Model Verification *(H)*** | **Characterization *(M)*** |
|---|---|---|
| *Need capability to predict reaction properties*<br>• *Kinetics*<br>• *Transport*<br>• *Physical/chemical*<br><br>*Expand molecular modeling capabilities to elucidate*<br>• *Solvation effects*<br>• *Bond order reactivity*<br><br>*Need to tighten integration of theory, experiments and simulation* | *Need new novel reactor systems which can be tested at laboratory scale*<br><br>*Need to use data taken under plant-scale conditions for model verification*<br><br>*Develop systematic method for measurements*<br>• *Standardize techniques*<br>• *Fine-scale CFD modeling*<br><br>*Develop experimental techniques for opaque flows, steel reactors, and large-scale reactors* | *Need better procedures for characterizing and cross- correlating the operational behavior of laboratory, pilot and plant scale reactors*<br><br>*Need simpler, cheaper, more robust equipment*<br><br>*Need new online techniques for tracking*<br>• *Local flow components*<br>• *Phase fractions for multiphase flows*<br>• *Composition*<br>• *Temperature* |

recycled through catalytic processes, and some will be sequestered. There will be some shift to natural gas and light alkanes, although alternative energy sources with lower $CO_2$ emissions will be found. The industry will likely use cogeneration as a primary tool for improving energy efficiency, together with the much broader use of methanol- or oil-based fuel cells. The use both liquid and gaseous hydrocarbons feed stocks will be limited to "high-value-added" products. There will be a continuous search for new feedstock with an attendant trend toward more plentiful C-1 candidates.

Safety will still be paramount, but chemical processes will be optimized to operate safely at more extreme conditions. Environmental concerns will likely be elevated to that of today's safety standards. Design methods for multifunctional reactors will be developed and these will be in common use in industry. Dynamic and model-based control, as well as non–steady-state processes, will be commonly used. Low inventory is expected, while more productive use of capital will be of increasing importance. Recycling will increase, and the current upward trend in plant size will continue. Theoretical and simulation methods will be used in catalyst design. The use of biocatalysis and electrochemistry will increase.

Advances in reaction engineering will lead to better product properties in high-volume chemicals. New intra-sector combinations will allow design of advanced products, in terms of structure–process relationship, by linking computational chemistry with chemical process engineering.

Existing tools, including experimental and computational tools, are not integrated, and are, therefore, often not optimally used. Capability improvements and increased integration of these tools are expected to play a key role in bringing them into more widespread use in the basic chemicals industry. Simulation tools are expected to improve computer-aided pilot-plant design/operation, and computer models will be integrated with experiments. Pilot-scale runs will be less extensive, being focused instead on the characterization of specific elements of the process identified by modeling as critical. New reactor designs, influenced by computational fluid dynamics will be more efficient, reliable, and safe. Computers will be faster and their interface with processes will be better, leading to more efficient automated control of integrated processes.

**Barriers:** Several areas have been identified where technical barriers exist which threaten to prevent or slow down innovations in reaction engineering. Technical barriers that were identified and prioritized are as follows: (a) Lack of online measurement techniques that allow experimental model verification under projected operating conditions is a barrier to further analytical and modeling advances. Similar limitations in both laboratory and real-plant characterization methods act as a weakness in systematic scale-up efforts. (b) Limitations in our ability to predict physical, chemical, kinetic, and transport properties of molecules, including polymers and long-chain organic molecules, is also a barrier to reactor characterization scale-up and design. (c) Often, the lack of understanding of complex chemical pathways and contactors/reactors inhibits advancements in this field especially in systems involving multiphase reaction environments.

A key research-related technical barrier is the segregation of disciplines, which characterizes our current chemical and chemical engineering education. As a result, the current engineering curriculum is insufficient in fundamental physics and chemistry while the chemistry curriculum is inadequate with regard to the importance of transport issues and rate processes. More recently, the rising emphasis on computer models has raised a problem of over-reliance on models to the point that they are often used beyond the range of their validity and without being tested against common sense thinking and historic knowledge. The risk and expense of implementing new technologies also poses a major inertial barrier in spite of the acknowledged high cost of existing experimentally based methods.

**Research Needs:** The following R&D needs were identified and prioritized in the order they appear below.

*Experimental Verification of Reactor Models:* New ideas for novel reactors are needed. Better characterization of both laboratory-scale and full-scale reactors is required. Collaboration should be encouraged between modelers and experimentalists for the generation of model input and experimental verification of reactor models. Fine-scale measurements for computational fluid dynamics verification are important. Plant data for model refinement should also be used.

*Ability to Determine Properties:* The ability to determine physical and chemical, kinetic, and transport properties of real and complex molecules, including polymers and long-chain organic molecules, needs to be improved. Quantum chemical and molecular simulation techniques need to be adapted and coupled to experimental measurements so as to enhance current predictive capabilities.

*Better Tools for Characterization of Reactors*: Better tools are needed for reactor characterization. These tools have to be simple, robust, cheap, and more accurate for detailed measurements. Such tools are especially needed for multiphase reactors where existing characterization techniques and modeling strategies are particularly limited. Fast response lab analytical techniques need to be hardened for use on operating plant-scale reactors. Non-visual reaction tracking methods for extreme reactor conditions are also needed.

*Research-Related Needs*: Adjustments in the educational system are also needed in order to meet the 2020 goals. Interdisciplinary training is needed to assure effective communication among team members having different backgrounds. A five-year BS program in chemistry and chemical engineering may be needed to achieve interdisciplinary training. Incentives and resources should be provided for the development of interdisciplinary courses. Also, interdisciplinary team projects should be encouraged early in the educational system. Faculty should be encouraged to gain industry experience so as to keep updated with current industrially significant reaction engineering problems.

# III.B. Specialty Chemicals

**Summary:** Technical experts in reaction engineering identified the top research needs for specialty chemicals to be (a) development of models to predict product properties *a priori* and for reactor/process design, and (b) increasing reaction selectivity. The key research needs are listed in Table III.B.1, while the complete list of prioritized barriers and research needs are provided in Tables C.B.1 and C.B.2 in Appendix C.

**Situational Analysis:** Specialty chemicals represent a wide diversity of high value-added products that are generally produced in relatively small volumes. These products are usually end-use/applications-oriented, and often have a short life cycle (ca. five years). Examples of products in this category include cosmetics, fragrances, consumer items, electronics manufacturing chemicals, water-treatment polymers, sealants, polymer modifiers, reactive monomers, specialty polymers, adhesives, oil additives, and surfactants.

The area of specialty and custom chemicals has distinct characteristics that differentiate it from other categories such as commodity chemicals and petrochemicals; pharmaceuticals, biochemicals and agricultural chemicals; and polymers and polymer intermediates. Unlike producers of large-volume chemicals, specialty chemical manufacturers must be more agile, and the cost of production is more important than for pharmaceutical producers. Companies generally produce many specialty products using the same equipment. Because of the scale of production, batch reactors are very common, with continuous processes used for some higher-volume precursors.

Specialty chemical companies are continuously driven to improve current products and to make new ones. Development generally follows the progression from laboratory research to pilot plant studies to manufacturing plant operations; however, due to constraints of time and money, there is increasing pressure to minimize or bypass pilot-scale work. However, this is difficult due to limited tools for understanding interactions of transport and chemistry in scale-up.

Processes used for production of specialty chemicals are not optimized to nearly the extent of commodity chemicals. In this competitive area, it is important to get the product to market quickly, often using existing equipment and optimizing the production process later, if justified. There are at least two challenges presented by this situation: developing a viable process while skipping some of the classical steps of scale-up, and determining the cost-effective level of optimization.

There is good projected growth for specialty chemicals in general. It is expected that U.S. companies will maintain some hold on their current leadership position, playing a continued significant role in 2020. The specialty chemical market will be increasingly customer driven. Since there is a semi-infinite number of chemicals that can be produced, it is very difficult to predict the major products of 2020. Specialty chemicals manufacturers will follow the needs of emerging new technologies (e.g., fuel cells, next-generation computers, pharmaceutical precur-

**Table III.B.1**
**Key Research Needs for Specialty Chemicals**
(H = High Priority, M = Medium Priority)

| Fundamental Science and Data | Reactor Design | Characterization |
|---|---|---|
| *Develop more sophisticated simulation models which can* ***(H)***<br>• *Predict product properties a priori*<br>• *Facilitate reactor/process selection*<br>• *Facilitate simultaneous catalyst/ reactor design*<br>• *Enable "virtual" process optimization* | *Increase reaction selectivity via* ***(H)***<br>• *Biochemistry, enzymes, biomimetics*<br>• *Catalysis, biocatalysis*<br>• *Combinatorial chemistry*<br><br>*Design efficient reactors* ***(M)***<br>• *Good understanding at small scale*<br>• *Novel reactors* | *Improve chemical sensors* ***(M)***<br>• *Cheap*<br>• *Reliable*<br>• *Nonintrusive* |

sors) and will adapt to provide the chemicals desired by the new markets. There will almost certainly be a drive toward increasingly more complex chemistries.

An idealized picture of 2020 for the specialty chemicals industry would include zero waste emissions. Although this will likely not be realized, some major steps could be made toward reusing byproducts. The byproduct of one process is often a valuable source material for some other product. In order to make use of byproducts, we will need a byproduct market network, with an information system capable of identifying opportunities.

**Barriers:** The main barriers to improvements in specialty chemical processes are both technical and business-related. There is room for significant technical improvement; more R&D would be performed if it were better, faster, and more cost-effective to do so. Technologies such as in-line sensors, rapid screening tools for kinetics (e.g., combinatorial chemistry), coupling computational fluid dynamics with lab kinetics data for scale-up, and ways to turn analytical information into accessible knowledge will improve the payoff of R&D. However, there is a lack of standard methods for applying life-cycle analysis to justify economic investment/improvements. Therefore, an opportunity for improvement exists through quantifying optimization payback, considering both the cost of optimization and the savings of optimized processes.

**Research Needs:** Modeling and information technology will have a significant impact in overcoming technical barriers. A major improvement envisioned for 2020 is the development of models for design of processes based on desired product properties. These models will provide a systematic means for predicting product qualities and performance from chemical structure, calculations, etc., to aid in the discovery process. The models will link to proprietary and open literature data on chemistry, catalysis, and reactor models to create virtual reactors/processes. Combinatorial approaches will be enabled, and process screening and optimization will be made through incorporation of materials and cost constraints as well as market drivers. Such models will guide laboratory work based on the desired product qualities, define and minimize laboratory confirmation tasks, and ultimately provide recommendations on process size and configuration.

The industry in 2020 will also have improved process technologies. Miniaturization, such as reactors on chips, will facilitate laboratory-scale work, and may result in a prevalence of small-scale continuous processing. Combination reactors, such as reactor/separators, will achieve greater efficiency. Improved, cheaper, robust sensors and instrumentation will allow greater understanding and control of processes. Modes of manufacturing may change; for instance, products may be manufactured in-process in portable reactors. "Magical" lab/pilot plant technology faithful to manufacturing reactor/process and improved methods for process definition/scale-up will provide methods to go directly from lab to manufacturing in many cases. Full-scale processes will use equipment that is more flexible than the conventional large batch reactor, perhaps through multiplexing of well-understood reactors of smaller scale.

The main target areas for improving performance in specialty chemicals are predicting product quality and performance *a priori*, improved process synthesis (predict best reactor process by virtual process optimization), validated models of processes, increased selectivity, sustainable operations, faultless processes (need perfect knowledge of chemistry and transport processes; avoid waste production, minimize consumption; recognize cradle to grave societal costs), improved process technologies, improved sensors, and alternative and/or novel reactors.

# III.C. Pharmaceuticals

**Summary:** Technical experts in reaction engineering identified the top research priorities for the pharmaceutical industry to be: (a) better experimental screening techniques to reduce development time and costs, (b) combinatorial techniques to evaluate synthesis, (c) thermochemical and thermophysical property data for complex systems, (d) better catalysts, and (e) improved reactor design for high purity, selectivity, and yield. The key research needs are listed in Table III.C.1, while the complete list of prioritized barriers and research needs are provided in Tables C.C.1 and C.C.2 in Appendix C.

**Situational Analysis:** The nature of pharmaceutical chemicals is that they interact with the human body. These chemicals typically resemble or mimic natural molecules. The most effective ones are readily available, safe, and easy to administer. These molecules may be small or large peptides, mimicking a protein, polysaccharide, or antibody. They often have chiral centers.

Smaller size (molecular weight <1000) pharmaceuticals make up approximately 90% of the existing pharmaceutical sales and typically require multistep organic synthesis to manufacture. These tend to be better messengers; they have higher permeability, are more tunable or easily modified, are more stable, are more soluble, and have higher diffusion coefficients. The remaining 10% of sales are derived from larger bioactive molecules derived from cell culture/fermentation. These molecules are typically too complex for traditional organic synthesis. Components in vaccines and therapeutic proteins with high

**Table III.C.1**
**Key Research Needs for Pharmaceuticals**
(H = High Priority, M = Medium Priority)

| Discovery Stage | Product Synthesis | Process Development | Plant Operations |
|---|---|---|---|
| *Develop better screening techniques* ***(H)*** | *Develop better catalysts to improve specificity* ***(H)*** | *Design improved reactors* ***(H)***<br>• *High purity, easily separated product*<br>• *High selectivity*<br>• *High yield* | *Develop robust scheduling tools for batch processes* ***(M)*** |
| *Develop better combinatorial techniques to evaluate synthesis options* ***(H)*** | *Develop methods to determine thermochemistry and properties data more precisely* ***(H)***<br>• *Chiral compounds*<br>• *Isomers*<br>• *Nucleation/crystallization* | *Reduce time and cost for process development* ***(H)***<br>• *Revamp registration process*<br>• *Cross-disciplinary training*<br>• *Better resource management tools*<br>• *Model development cycle to manage personnel and risk* | *Develop highly selective, durable, online instrumentation* ***(M)*** |
| *Improve experimental design to reduce cost and time requirements* ***(H)*** | *Develop highly selective, durable, online instrumentation* ***(M)*** | | *Develop cheap, easily applied sterilization processes* ***(M)*** |
| *Develop fundamental models for synthesis chemistry and entire system****(M)*** | *Understand solvation effects* ***(M)*** | *Understand solvation effects* ***(M)*** | |

binding specificities are examples. The surge in biotechnology is focused primarily on these.

Drug discovery starts with an understanding of the nature of a disease. Understanding the mechanism of a disease leads to an assay or simulation; this in turn allows the development of a screening process in which the prospective pharmaceutical is produced on a small batch scale and tested against the disease.

Batch reactors are the norm for full-scale production of pharmaceuticals. These reactors can typically take multiple feeds, are easy to clean, and rarely require specific reactor design modifications. Sometimes highly exothermic reactions require special precautions, but these are uncommon. Continuous reactors are only used in special cases, such as when very fast reactions are involved.

Production volumes vary considerably. Typical ranges are 100 to 2000 gallons capacity, with product levels as high as 500 kg per batch. Most reactors typically operate between –70 and 150 °C. Stoichiometric considerations are generally limited by the most expensive reactants. Twenty percent of processes involve catalytic reductions—mostly liquid phase with solid catalysts. A small fraction of catalysts are homogenous and enantioselective, having the advantage of high selectivity and yield. There may be 8 to 15 steps involved in making a product, with a typical step yield of 85%. Reactions are usually one-way, rather than having equilibrium limitations. Pharmaceutical processes tend to generate very dilute solutions that require complex separation steps (including chromatography) for recovery of intermediate and final products. Proper selection of solvents is important for maintaining the purity of the final product.

A diagram of the current sequential pharmaceutical development process is shown in Figure III.C.1. The length and complexity of the reaction synthesis has a major impact on the cost of pharmaceuticals. If steps could be either omitted or simplified, it would have a dramatic effect on the costs. These improvements are generally made by altering the chemistry of the process. If new separation techniques could be employed, then production costs can also be lowered since these tend to be a large percentage of the total cost (perhaps 80% or more).

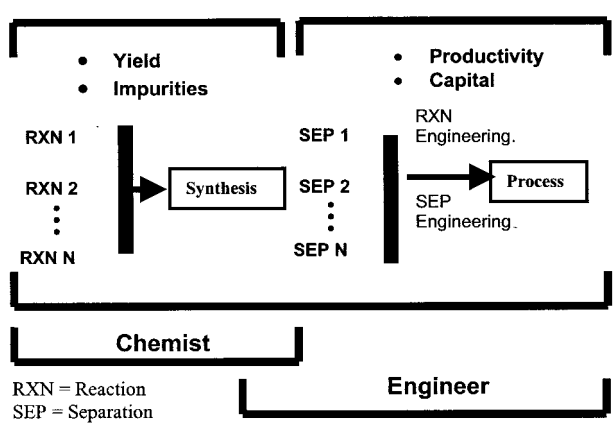



**Figure III.C.1. Current sequential process for pharmaceutical development**

To improve the process as much as possible, engineers and chemists must collaborate through all phases of the process, and work together closely. Process engineering must be considered during synthesis and vice versa.

Raw materials costs, time required for development, and capital costs are also factors that will influence the pharmaceutical industry in the future. Speed is becoming more and more important, especially as the Food and Drug Administration begins to give drug approvals in less than a year. Better integration of the manufacturing process will be essential in 2020. Better coupling of synthesis and separations will be prominent in the future. This will be particularly true for chiral separations. These hybrid processes will simplify reaction and make better use of materials. For example, existing racemic syntheses requiring four steps may be condensed into a single step in the future. Although we will have better control of each reaction step, reaction mechanisms will still limit the number of processing steps.

Innovative solvents will be more prominent by 2020. There will be more use of aqueous solvents, more consolidation of nonaqueous solvents, and fewer solvents used in general (which means fewer recovery steps). Use of safer reagents will be more common. Syntheses may be redesigned to reduce the quantities of toxic materials produced. Impurity control will be very important. Currently, allowable impurity levels are typically set at 1000 ppm (or 0.1 %).

There may be much better software for better pharmaceutical design and production. Multipurpose pharmaceutical factories will be the norm. For instance, a plant might produce one drug continuously for one month, then switch modes to manufacture a different drug. Pilot plants will still be essential, since these generate the clinical supplies needed for testing approvals. This differs from commodity chemical production, which may be able to bypass pilot production using advanced design tools.

For pharmaceuticals, there are two sustainability indicators that should be added to the list discussed in Section II: (a) return on investment for equipment, and (b) speed to market. Most reactors in the pharmaceutical industry are glass-lined batch reactors. There is not a huge incentive to change to more complex reactor types. And, although multifunctional, multicomponent feedstocks are desirable in general, feedstock costs are not typically drivers for pharmaceutical syntheses. Speed to market is essential. Water usage, listed as a sustainability indicator in Section II, is not a cost driver for pharmaceuticals since batches are small (a few thousand gallons) and infrequent (two or three per year). Energy requirements to heat, cool, or sterilize equipment during operation are not significant for this industry. For systems that require multistage, sterile processing, however, sterilization costs may be an important factor.

**Barriers:** There are currently several high priority technical barriers that will impact advancements in reaction engineering in the pharmaceutical industry. The first is a lack of effective reaction modeling tools. There is presently no method to model synthesis for the reaction system as a whole. There is also a lack of catalysts to perform these syntheses efficiently. Selectivity of pharmaceutical separation processes can be very low. There is a lack of high-speed reaction/synthesis screening tools to predict impurities in products. There is also a lack of fundamental understanding of chemical systems involved in the production of pharmaceuticals. This includes thermophysical properties, mechanisms, chiral processing, and solvent effects. Bioreactors for novel products are rare, and their designs are presently too simplistic.

Research-related technical barriers include the lack of cross-disciplinary training of chemist and chemical engineers at universities. The simultaneous regulation of products and processes limits development opportunities. Once a product goes into clinical testing, its process is fixed and can no longer be modified without revalidating it with further clinical tests.

**Research Needs:** The group identified high priority research needs and categorized them by stages in the drug development process:

*Discovery*: High priority research needs include better screening tools and more efficient experimental designs to speed up the drug development process. Concurrently, better combinatorial techniques are needed to evaluate potential synthesis routes.

*Product Synthesis:* Better catalysts are needed to improve the specificity of synthesis. More precise thermochemical property data are needed for complex systems such as chiral compounds, isomers, and nucleation/crystallization. Better instruments are needed to monitor and control the synthesis process.

*Process Development*: New reactor designs are needed to improve selectivity, yield, and solvation. Of special interest are designs that integrate the reaction and separation steps.

*Research-Related Needs:* Cross-disciplinary training of biologists, chemists, and chemical engineers is needed at universities. Changing the regulatory process to decouple regulations on product and the production process would allow for innovation.

# III.D. Polymers and Polymer Intermediates

**Summary:** Technical experts in reaction engineering identified the top research priorities for the polymers industry to be: (a) better experimental screening techniques to reduce development time and costs, (b) advanced property prediction capabilities, (c) the ability to link process conditions to product properties (at the micro-, meso-, and macro-scales), and (d) designing polymers that can be disassembled (unzipped) for recycling. The key research needs are listed in Table III.D.1, while the complete list of prioritized barriers and research needs are provided in Tables C.D.1 and C.D.2 in Appendix C.

**Situational Analysis:** At the present time, industry is focused on making new polymers with better properties. Today this is primarily done by developing new catalysts to make polymers with new microstructures. Reactor designs have not changed significantly over the last 30 years. This trend must change in the future for the industry to remain competitive.

The future market for polymers is expected to grow significantly if the public perceives the industry to be environmentally friendly. In order to achieve this, toxics (chlorinated solvents) should be eliminated, and polymers will need to be recyclable. The trend towards full life-cycle product ownership will continue. Water reuse will also be important in the future. This will result in an increased need to convert to nontoxic solvents and/or solventless processes. Feedstocks are likely to change from petroleum-based to gas and/or bio-based feed stocks (wood, cotton, etc.) and carbon dioxide. Processes will need to be developed to deal with the variability in the new bio-based feedstocks and the need for more stringent quality control on products. New computational methods will be needed to achieve these objectives and to bring new products to market in an economical, timely manner. Corporate decisions are likely to be based much more on total cost accounting and sustainability evaluations in the future.

New specialty polymers will be developed in the future which have vastly different microstructure properties. The improved properties, which will result, will enable these polymers to replace energy-intensive materials in many applications—such as steel, wood, and other building materials; vehicle applications—and to have new uses, such as drug encapsulation, electro-optical materials, and prosthetics.

**Barriers:** There are several technical barriers that must be overcome to achieve the future potential of the polymer industry. These include inadequate raw material supplies and processing capabilities. Existing computational tools are lacking in their ability to design polymers and catalysts. To support these models, there needs to be a better understanding of the interaction between properties, structure, and the process by which these polymers are manufactured. In order to recycle polymers, materials must be depolymerized, or unzipped. The development time required to bring new processes on line and new products to market needs to be significantly reduced.

**Research Needs:** The group identified high-priority research needs and categorized them as follows:

**Table III.D.1**
**Key Research Needs for Polymers**
(H = High Priority, M = Medium Priority)

| Modeling | Materials Development | Processing |
|---|---|---|
| *Develop advanced combinatorial methods for polymer property screening* ***(H)*** | *Design new recyclable polymers* ***(H)*** | *Need better models to connect process conditions and polymer product properties* ***(H)*** |
| *Need better advanced property prediction capabilities* ***(H)***<br>• *Infrared*<br>• *Materials strength* | *Design catalysts to disassemble existing polymers for recycle* ***(H)*** | • *Link micro-scale to meso-scale to macro-scale properties*<br>• *Understand interaction between properties, structure, and performance*<br>• *Understand catalyst and polymer design* |
| *Need fundamental-based reactive computational fluid dynamics models for simulating large molecule reaction environments* ***(M)*** | | *Need online monitors for in situ property measurement and reactor analysis* ***(M)*** |
| *Need models to control spatio-temporal gradient patterns in reactors* ***(M)*** | | *Develop novel ways to combine reactions and separations* ***(M)*** |

*Modeling:* Better computational methods are needed to allow predictive design of polymers and catalysts. A fundamental understanding of the relationship between reactor operating conditions and product properties at all levels (micro-, meso-, and macro-scales) is needed to support these models and improve process operations. New computational fluid dynamic models are needed for the complex viscous flow systems involved in reactions of large molecules. Models are also needed to control spatio-temperal gradients in reactors. Needs include faster computers, more accurate algorithms, accurate semi-empirical parameters for model input, experimental data for model input and validation, multiscale approaches, and ultimately, fundamentals-based approaches.

*Materials Development:* New polymers need to be designed that can later be broken down to monomers on demand to facilitate recycle. New catalysts need to be developed to facilitate depolymerization, or unzipping, of existing polymers for future recycle. Better experimental screening methods need to be developed to reduce development time and costs.

*Processing:* Online monitors are needed for property measurements and reactor characterization. The need is to measure chemical and materials properties, such as Fourier Transform Infra-Red, material strength, spectra, and nuclear magnetic resonance. They can also be used for advanced process control once reactor operations can be linked to materials properties.

Novel methods are needed to combine reactions and separations in one step. These include reaction injection molding, reactive extrusion, reactive separations, and transport phenomena.

# IV. TECHNOLOGY SEGMENT RESEARCH NEEDS

## IV.A. Reactor Design and Scale-up

**Summary:** Industrial experts in reaction engineering identified the top priority research needs for reactor design and scale-up to be: (a) physical/chemical and transport property data for input into and verification of models, and (b) development of robust models for reactor design and synthesis development. The key research needs are listed in Table IV.A.1, while the complete list of prioritized research needs are provided in Table C.E.1 in Appendix C.

**Situational Analysis:** The traditional scheme for reactor system selection, design, and scale-up has been laboratory-scale development to pilot plant testing to full-scale production. Throughout this progression, a range of activities involving varied skills is employed. At the laboratory scale, process R&D involves such tasks as chemists modeling and synthesizing new compounds, engineers assessing processing alternatives, and financial analysts evaluating profitability. At the pilot scale, process engineers translate bench research into small-scale processes, test and validate process approaches, and redesign and adapt as necessary. In the transition to production scale, engineers further test and adapt processes, validate performance at full scale, and perform operator training and process documentation.

The key elements in process selection and scale-up may be summarized as:

1. Synthesis of alternatives
   - ♦ reactor synthesis
   - ♦ verification
   - ♦ detailed design
2. Evaluation of alternatives
   - ♦ economics
   - ♦ safety
   - ♦ environment
   - ♦ quality
   - ♦ controllability
3. Resource allocation to reduce
   - ♦ experimentation
   - ♦ pilot plant operation
   - ♦ uncertainty
   - ♦ development of new models
   - ♦ manpower required
4. Performance optimization
5. Construction of reactor systems.

Generally, extensive pilot-plant testing is not currently undertaken for systems for which a large experience base exists and/or for which there are trusted models. Some examples are liquid-phase reactors, tubular reactors, fixed-bed reactors, trickle-bed reactors, and some fluidized-bed reactors. On the other hand, demonstration-scale pilot testing is vital for multiphase reactors and nearly all reactors for which heat transfer and/or mixing effects are important.

Throughout the chemical industry, a uniform desire is to make process scale-up faster and cheaper. However, full-scale designs must be robust and of high quality. It is necessary to obtain sufficient information on new products or processes prior to scaling up to avoid economic loss and possibly significant safety problems.

The main sustainability performance goal in reactor system selection, design, and scale-up for 2020 is to reduce the number of development steps used to move from the lab to commercial production. Attaining this goal will improve performance in two ways: (a) the amount of resources spent and waste produced during scale-up will be minimized by reducing the number of testing stages, and (b) the improved process synthesis/design methods will produce more efficient processes.

**Research Needs:** To meet the future goals of reactor design and scale-up, progress is needed in a number of areas: fundamental data, modeling, experimental tools, processing, and education.

The improved process models of the future will be integrated, validated tools that span all size scales. Such models will incorporate fundamentals of chemistry, reaction kinetics, and transport processes. They will capture the complexity of real systems at fine scales; this will be particularly important for multiphase systems that are currently extremely difficult to scale up. By incorporating

**Table IV.A.1**
**Key Research Needs for Reactor Design**
(H = High Priority, M = Medium Priority)

| Need Category | All (Ongoing Processes) | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Fundamental Data and Science*** | *Data for validation of models across multiple scales* ***(H)***<br><br>*Capture uncertainty variability in measurements of data used in models* ***(H)*** | *Obtain better characterization of lab-scale reactors for obtaining kinetic data* ***(H)***<br><br>*Obtain thermochemical and transport property data for complex systems such as chiral isomers* ***(H)*** | *Develop laboratory reactors for synthesis of specific complex chemistries* ***(H)***<br><br>*Obtain thermochemical and transport property data for complex systems such as chiral isomers* ***(H)*** | *Develop micro-reactors for obtaining experimental design and modeling data* ***(H)*** |
| ***Experimental Tools*** | | | *Develop accelerated methods to predict catalysts deactivation and time-dependent product properties* ***(M)*** | *Develop methodology to accelerate the scale-up of processes including redefining the role of pilot scale* ***(M)*** |
| ***Processing*** | *System optimization* ***(H)***<br>• *Scheduling*<br>• *Parameter estimation*<br>• *Experimental design*<br>• *Risk/resource management*<br><br>*Improved sensors* ***(M)***<br>• *Cheap, reliable chemical sensors* | *Improved sensors* ***(M)***<br>• *Advanced instrumentation strategies* | *Improved sensors* ***(M)***<br>• *Advanced instrumentation strategies*<br>• *Smart tracers for in situ, real-time measurement of composition, temperature, flow, pressure, & telemetry* | *Improved sensors* ***(M)***<br>• *Smart tracers for in situ, real-time measurement of composition, temperature, flow, pressure, & telemetry* |
| ***Modeling*** | | *Develop models of reactions with mixing and transport* ***(H)***<br>• *Scaling tools*<br>• *Property prediction*<br><br>*Develop reactor synthesis models* ***(H)***<br>• *Geometry*<br>• *Heat & mass transfer*<br>• *Materials selectivity*<br>• *Trace products*<br>• *Separations* | *Develop models which incorporate chemistry, kinetics and transport at a more fundamental level* ***(H)***<br>• *Scaling tools*<br>• *Property prediction*<br>• *Develop tighter integration of theory and experiment into models*<br>• *Improve model precision to incorporate more detail on side reactions and trace impurities* | |

detailed reaction chemistry and transport, the models will determine selectivity and even predict production of byproducts at trace levels in side reactions. Integrated modeling of reactions and separations will provide complete reaction and reactor synthesis tools suitable for systems-level assessment of safety and economics. Modeling will also help to determine the value of various types of information, providing a measure of sensitivity, reliability, and uncertainty in process measurements.

The models of the future cannot be developed without experimental verification. Modelers and experimenters need to work together to obtain needed knowledge and capability. New ideas for lab reactors are needed to improve the efficient collection of complete and accurate kinetic data. Better characterization of lab-scale and full-scale reactors is needed, coupled with a better understanding of the effects of transport phenomena on reaction processes. A key for improving the understanding/characterization of processes at various scales is the

development of cheap, reliable chemical sensors. It is highly desirable to develop monitors/sensors for in situ, real-time measurement of composition, pressure, flow, temperature, etc. with accompanying telemetry data. Accelerated property testing will also be a key feature in experimental/modeling progress. Improved methods for determining and predicting catalyst deactivation and time-dependent product properties (e.g., quality and stability) will greatly advance process efficiency and reduce waste.

A research-related need is improved education. This is perhaps nowhere seen more plainly than in process scale-up, where a multitude of skills is necessary. In the future it will be increasingly important for engineers to have an integrated knowledge of chemical systems and design tools, and for chemists to have a deeper awareness of plant-scale transport issues. This may entail a five-year BS education in both disciplines. Equally important will be improved interaction between industry and academia, including industrial experience programs for faculty and scholarships/fellowships for visiting scholars from industry.

# IV.B. Chemical Mechanisms

**Summary:** Technical experts in reaction engineering identified the major research priorities for chemical mechanism development to be (a) micro-kinetic experimental capabilities, (b) methods to integrate solvent effects into reaction models, (c) tools to couple process chemistry and process modeling, and (d) methods to determine macroscopic properties from molecular structures. The key research needs are listed in Table IV.B.1, while the complete list of prioritized research needs are provided in Table C.F.1 in Appendix C.

**Table IV.B.1**
**Key Research Needs for Chemical Mechanisms**
(H = High Priority, M = Medium Priority)

| Need Category | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|
| ***Experimental Tools*** | *Develop accessible microkinetic experimental capabilities* ***(H)***<br>• *Heterogeneous catalysis*<br>• *Multiphase systems* | *Better sensors* ***(M)***<br>• *Fast response to track transient species*<br>• *Online analyses*<br>• *Multi-species*<br>• *Multiphase* | |
| ***Mechanism Capabilities*** | *Improve precision of electronic structure methods to calculate reaction rate parameters, transition states and heats of reaction* ***(M)*** | *Develop methods to integrate solvent effects into reaction models* ***(H)***<br>• *Especially for weak forces*<br><br>*Expand mechanism development methods* ***(M)***<br>• *Electrochemical processes*<br>• *Photon processes*<br>• *Plasma-driven processes* | |
| ***Mechanism Inputs*** | *Develop models with surface species migration and reaction under full range of process conditions* ***(M)***<br><br>*Obtain thermophysical, thermochemical, and kinetic data for property models* ***(M)*** | *Obtain thermophysical, thermochemical, and kinetic data for property models* ***(M)*** | *Develop theoretical and experimental methods for macroscopic properties from molecular structures* ***(H)*** |
| ***Mechanism Development Tools*** | *Couple process chemistry models with experiment to elucidate understanding* ***(M)*** | *Develop practical tools which couple process chemistry with process modeling* ***(H)***<br>• *Better use interface*<br>• *Better software integration*<br>• *More robust numerics* | |

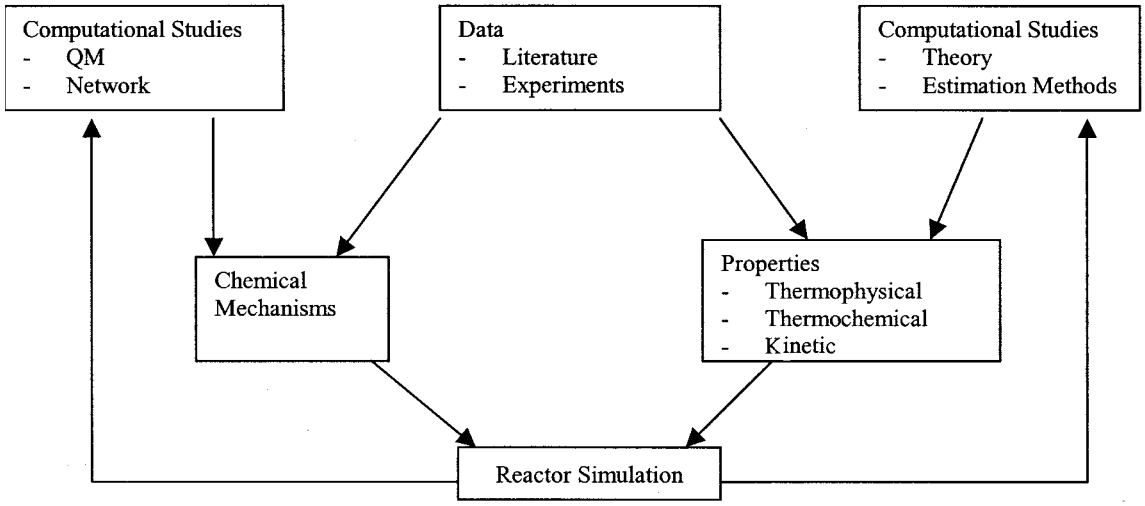



**Figure IV.B.1. Process for chemical mechanisms development.**

**Situational Analysis:** Figure IV.B.1 shows that the process for development of chemical mechanisms is an iterative, interactive one. Computational results, literature data, and experimental information are used to determine the chemical mechanisms and thermodynamic and transport properties. This information feeds into reactor simulation models. The model output is compared to actual reactor data, and used to modify the computational models. In order to perform chemical mechanism development effectively in the future, each of these areas needs improvement. In addition, the interface between areas must be enhanced.

Experimental data (as well as online analytical tools to obtain the data) are needed for input into and validation of models. Faster more efficient methods are needed for evaluating data and converting existing data into useful inputs for computational tools. Better mechanism development tools are needed, and better mechanism discrimination (or reduction) tools are needed. Existing tools are not powerful enough, not fast enough, and require too much specialist knowledge. Reliable, efficient numerical tools with good user interfaces are needed. Programs similar to ASPEN, but built on realistic molecular science, can be envisioned for the future. More effective tools need to be developed to couple the process chemistry with the process modeling at the micro-, meso-, and macro- scales. Experimental design, user interface, software integration, and numerical methods must all work closely together to develop an efficient system that will improve reaction engineering.

**Research Needs:** The research needs associated with chemical mechanisms were grouped into four technical areas and prioritized: experimental tools, mechanism capabilities, mechanism inputs, and mechanism development tools. The high priority research needs primarily deal with development of models to predict chemical mechanisms:

- development of accessible microkinetic experimental capabilities to obtain data for models (particularly for heterogeneous catalysis),
- development of methods to integrate solvent effects into reaction models,
- development of practical tools to couple process chemistry with process models, and
- development of theoretical and experimental methods to obtain macroscopic properties from molecular structures.

Medium priority research needs included development of models with surface species under the full range of process conditions; obtaining thermophysical, thermochemical, and kinetic data for input into properties models; and development of fast, accurate online sensors for multiphases and multispecies to track transient intermediates at laboratory and plant scale. More accurate electronic structure methods need to be developed to calculate rate parameters, transition states and heats of reaction. More reliable automated procedures are needed for pathway analysis and pruning rules in both forward and reverse directions. Mechanism development methods should also be expanded to include electrochemical, photon-, and plasma-driven processes.

# IV.C. Catalysis

**Summary:** Technical experts in reaction engineering identified the major research needs for catalysis to be (a) better in situ characterization and synthesis methods, (b) system integration techniques to optimize catalyst and reactor design and operations concurrently, (c) catalysts for solid matrices, and (d) fuel-cell-related catalysts. The key research needs are listed in Table IV.C.1, while the complete list of prioritized research needs are provided in Table C.G.1 in Appendix C.

**Table IV.C.1**
**Key Research Needs for Catalysis**
(H = High Priority, M = Medium Priority)

| Need Category | All (Ongoing Processes) | Near Term (0-3 Years) | Mid-Term (3-10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Chemistry*** | *Fischer-Tropsch synthesis* ***(M)***<br>*Mechanistic studies* ***(M)***<br>*Catalysis of alternative feedstocks* ***(M)*** | | *Fuel-cell-related catalysis* ***(H)***<br>*Stereo-selective synthesis* ***(H)***<br>*Selective oxidation* ***(M)***<br>*Catalyst support design* ***(M)*** | *Hydrocarbon activation* ***(M)*** |
| ***Experimental Tools*** | *Development techniques for high throughput screening and synthesis* ***(M)*** | | *Better in situ techniques for sensing and characterization at both bench and plant scale* ***(H)*** | *Detect transient intermediates* ***(M)*** |
| ***Processing*** | | *Advanced analysis tools and precise data screening (e.g. neural nets)* ***(M)*** | *System integration (laboratory): combining experimental tools and modeling tools to give kinetics and reactor design in integrated easy steps* ***(M)*** | *System integration (plant scale): Optimize both the catalyst and reactor at the same time* ***(H)***<br>*Fundamental understanding of plant-scale processes* ***(M)*** |
| ***Modeling Tools*** | *Based on fundamentals rather than empirical* ***(M)***<br>*Transport* ***(M)***<br>*Predicting catalyst life* ***(M)*** | *Develop better screening and design tools to accelerate development for new catalysts* ***(M)***<br>*Achieve better integration of models and experiment* ***(H)*** | *CFD with catalysts* ***(M)***<br>*More sophisticated prediction of product quality and performance a priori (model and validation)* ***(M)*** | *Develop models to predict life as well as performance* |
| ***Catalyst Design*** | *Attrition, coking, deactivation issues* ***(M)*** | *Contacting patterns between catalyst and reatants.* ***(M)*** | *Supercritical and subcritical catalysis* ***(M)***<br>*Increase selectivity for site-specific catalysts, biocatalysts, enzymes, biomimetics* ***(M)*** | *Design catalysts for applications involving solid matrices (e.g., coal, complex polymers)* ***(H)*** |

**Situational Analysis:** The *Vision 2020 Catalysis Report* has been completed, and a copy can be obtained from the DOE/OIT web page. The situational analysis and the research needs for the general chemical industry are summarized in that report. Research needs specific to reaction engineering are summarized below.

**Research Needs:** Catalysis research needs specifically required for reaction engineering were identified and categorized into five technical areas: basic chemistry, experimental tools, processing, modeling, and design. The highest priority research need was the development of better in situ techniques for sensing and characterization (both at the bench scale and for plant operations). Catalyst development for fuel cells was seen as the next highest priority. This was closely followed by the need for systems integration. At the laboratory scale, there is a need for combining experimental tools and modeling tools to yield kinetics and reactor design information in one combined step. At the plant scale, there is a need for integrated reactor system design to optimize the reactor operations and catalyst at the same time. Other high priority research needs include stereo-selective synthesis and design of catalysis for applications involving solid matrices (e.g., coal and complex matrix polymers). Access to chemical sites is limited in materials such as these.

Medium priority research needs for basic chemistry development include improved catalysts for processes involving selective oxidation, hydrocarbon activation, Fischer-Tropsch synthesis, and for enabling utilization of alternative feed stocks. Experimental tools needing development include techniques to detect transient intermediates (tightened temporal analysis of the reaction which is highly specific to intermediates), and techniques for high

throughput screening and synthesis. Processing needs include advanced analysis and precise data screening (e.g. neural nets) tools, and being able to extract fundamental information from plant data. Modeling tools are needed to reduce development time for new catalysts, using fundamental information in conjunction with experimental input. Models are needed which can predict catalyst life as well as product quality and performance. Catalyst design needs include developing materials for supercritical and subcritical systems; understanding contacting patterns between catalyst and process fluids; reducing attrition, coking, and deactivation; and increasing the selectivity for site-specific catalysts, biocatalysts, enzymes, and biomimetics.

Research-related needs included increased interdisciplinary training at the university level.

# IV.D. Novel Reactors

**Summary:** Development of new, nonstandard reactors is dependent on advances in fundamental research and enabling technologies needed to apply this to reactor design. Research areas include intensified reactors (in terms of energy efficiency, mass transfer, heat transfer, etc.), rapid heating and cooling, structured contacting, external field-assisted and photochemical reactions, and reactors for extreme conditions. Enabling technologies include new materials development, systems integration, micro-properties and phenomena determination, multistage design capabilities, and self-assembling reactor development. The key research needs are listed in Table IV.D.1, while the complete list of prioritized research needs are provided in Table C.H.1 in Appendix C.

**Table IV.D.1**
**Key Research Needs for Novel Reactors**
(H = High Priority, M = Medium Priority)

| Need Category | All (Ongoing Processes) | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Fundamental Data and Science*** | *Develop micro-properties and phenomena* ***(M)*** | | *Develop automated synthesis* ***(M)*** | *Develop artificial cells* ***(M)*** |
| ***Materials*** | *Better materials* ***(H)***<br>• *Extreme conditions*<br>• *Micro-fabrication*<br>• *Catalysts*<br>• *Sensors* | | | |
| ***Design*** | *Improve systems integration* ***(H)***<br>*Develop multiscale design capabilities* ***(H)***<br>*Develop self-assembling reactors* ***(H)***<br>*Develop intensified reactors* ***(H)***<br>*Develop structured contacting* ***(H)***<br>*Develop biomolecular design capabilities* ***(H)***<br>*Develop rapid heating/cooling systems* ***(H)***<br>*Develop external-field assisted reactions* ***(H)***<br>*Develop/demo photochemical reactors* ***(H)*** | *Develop ultra-low-cost reactors* ***(M)*** | *Develop fuel processors* ***(M)*** | |
| ***Demonstrate Value*** | | *Develop/demo immobilized cell and enzyme reactors* ***(H)***<br>*Develop reactors for extreme conditions* ***(M)*** | *Develop/demo electrochemical reactors* ***(H)***<br>*Develop/demo biomimetic reactors* ***(H)*** | *Develop/demo biomimetic reactors* ***(H)*** |
| ***Enabling Technology*** | | *Micro fabrication techniques for micro reactors* ***(M)*** | *Advanced materials for extreme condition reactors* ***(H)*** | |

**Situational Analysis:** The following properties have been identified as desired functionalities for the novel, or nonstandard, reactors of the future. Their capital cost has to be reduced, while heat and mass transfer characteristics have to be improved. Energy requirements should be reduced, while safety standards should remain high. Advanced knowledge of reactor operation should allow intensification of nonstandard reactors. In addition, nonstandard reactors should allow complete data acquisition and predictive modeling that would lead to better process integration and easier scale-up and miniaturization. They should be multifunctional, in terms of chemical reactions and separation, capable of producing ultrapure products. They should be versatile and controllable, and they should handle transient operation. Improved design methods should streamline reactor design contributing to reduced time-to-market.

Projected requirements in the fuels and energy industry include production of cleaner gasoline, as well as hydrogen and methanol. More renewable fuels will be produced, driven by requirements for lower emissions. Smaller and more modular reactors will be needed, while safety standards will be kept high. In the transportation industry, fuel cells, and especially fuel reformulation, will be important. In the basic chemicals and commodities industry, the requirements will be: higher selectivity and yield, less waste, less capital cost, less energy needs, and less emissions. The trend in feedstocks will be away from fossil fuels and toward broader use of more renewable bioderived fuels. More recycling will be practiced, and more biodegradable products will be produced. Safety standards will remain high. In the fine chemicals industry, reducing the time to market will be a driving force. Higher versatility, in terms of transferring the reactor technology to different processes, and higher purity will be very important. Also, how reactors are scaled up will be a determining factor in the development of nonstandard reactors. In the polymers industry, tailoring the properties of products with thermodynamic and transport properties of chemical reactors will be one of the driving forces for the development of novel nonstandard reactors. Product purity, ability to recycle a product, and ability to control the polymer microstructure will also be important in the development of nonstandard reactors. Tailored properties, microstructure control, solids handling, consolidation of process steps, will also be important in the development of nonstandard reactors for materials, catalysts, microelectronics, and ceramics industries. Similar to the fine chemicals industries, the time to market will play a significant role in the pharmaceuticals industry. The ability to trace the product/process will also be important. Chemical reactor innovations in this industry will be driven by discoveries of new products and new chemistries. Innovations in drug delivery systems will also play a significant role.

A summary of the desired functionalities of novel nonstandard reactors for various industries is shown in Table IV.D.2. The novel nonstandard chemical reactors for various industries, including fuels and energy, transportation, monomers, fine chemicals, materials, polymers, and pharmaceuticals, should have one or more of the following functionalities. They have to be multifunctional (e.g., contactors, reactors, separators) intensified (in terms of energy efficiency, mass transfer, heat transfer, etc.), robust (in terms of parametric sensitivity), scaleable at larger and smaller scales, modular, and inherently safe, and their performance should be predictable.

**Table IV.D.2**
**Desired Functionalities of Novel Reactors**

| Novel reactor | Commodities | Fine Chemicals | Polymers/ Materials | Pharmaceuticals |
|---|---|---|---|---|
| *Multiphase* | *X* | *X* | *X* | *X* |
| *Moving Bed* | *X* | | | |
| *Extreme Conditions (intensified)* | *X* | *X* | *X* | |
| *Versatile* | | *X* | *X* | *X* |
| *Information (micro-reactors included)* | *X* | *X* | *X* | *X* |
| *Multifunctional (membrane reactors included)* | *X* | *X* | | |
| *Transient* | | *X* | *X* | *X* |
| *High gradient* | | *X* | *X* | *X* |

**Research Needs:** Ongoing research needs identified for the development of novel nonstandard reactors include: intensified reactors, rapid heating and cooling, structured contacting, external field-assisted, photochemical reactors, and reactors operated under extreme conditions. For the next 3 years, research needs have been identified for the development of ultra-low-cost reactors (including disposable reactors) and immobilized-cell and enzyme reactors. Between 3 and 10 years, there will be research needs for automated synthesis, fuel processors, biometric reactors and electrochemical synthesis reactors. After 10 years, research will be needed for the development of artificial cells.

Technological advances in many fields will enable success of the research goals toward the development of novel nonstandard reactors. Advanced materials of construction will allow operation at extreme conditions, micro-fabrication in the development of small reactors, production of better catalysts and structured contacting devices, and fabrication of advanced sensors. Systems integration will lead to ultra-low-cost reactors and automated synthesis. Micro-properties and phenomena will enable the development of multiuse and multifunctional reactors, external-field-assisted reactors, as well as reactors with rapid heating and cooling capabilities. Multiscale design capability will enable rapid scale-up and scale-down to different sizes for different purposes. Large reactors will increase production, while small reactors may be used for either production or information. biomolecular design will allow the development of immobilized-cell/enzyme reactors, artificial cells, and biomimetic reactors. Self-assembly will also enhance the development of novel nonstandard reactors, including photochemical and electrochemical reactors.

New technologies that will emerge up to 2010 in the area of nonstandard chemical reactors will include reactors wherein multistep reactions and separations will be integrated into a "one-step source-to-pure-product" system. These reactors will feature several of the desired functionalities of chemical reactors that are currently identified, such as multifunctional, intensified, and ultra-low cost. After 2010, emerging technologies will make broader use of external energizing systems such as plasma, photochemical and electric fields. Broader use of non–steady-state reaction systems guided through prescribed model-driven cycles will also become common. Multistep microreactor systems with high-speed sensors both for the generation of detailed kinetic data and production of high value or high hazard materials will also become common.

# V. CROSS-CUTTING RESEARCH NEEDS

Major research needs were identified that cut across several or all of the technical areas. These fell into four technical categories: experimental tools, simulation models, sensors, and system integration.

**Experimental Tools:** Improved experimental tools are needed to design and optimize reaction engineering systems more efficiently and to provide input data for models. Better experimental screening techniques and more precise methods to predict product properties are needed to reduce development time. Cheaper and faster methods for generating detailed reaction information are needed.

**Simulation Model:** Improved models are needed to support design and operation of reaction engineering systems. Thermophysical, thermochemical, and transport data are needed for inputs into and validation of these models. Models need to be developed that are based on fundamental science rather than empirical fits to experimental data. They need to be able to address systems with multiple phases and components and with complex mass heat and momentum transport patterns.

**Sensors:** Fast, precise, robust, online sensors are needed for data collection, monitoring, and process control. Data collected will be used for experimental studies and as model input for bench-scale and plant-scale systems as well as for optimizing process control on plant systems.

**System Integration:** Integration of the research areas is required to develop useful tools for ndustry efficiently and effectively. There is a need for better integration of component models into a model of the whole process system along with experimental data gathering. Models need to be developed which couple process chemistry with process equipment models. Ultimately, design and optimization tools are needed which will link process conditions to product properties at the micro-, meso-, and macro-scales.

Research-related needs were also identified. They include institutional, regulatory, and educational issues. The major research-related needs identified include (a) the need to put more emphasis on interdisciplinary education at universities, and (b) the need to reduce the time and cost for bringing new processes on line and new products to market to remain competitive in the 2020 industrial environment.

# APPENDIX A
# WORKSHOP AGENDA

The Reaction Engineering Roadmap has been prepared based on the information gathered in a workshop held in conjunction with the 1999 Annual American Institute of Chemical Engineers' meeting in Dallas, Texas on October 30–31, 1999. The workshop brought together 46 experts from the chemical industry, its customer industries, universities, and government research laboratories to brainstorm on research needs for reaction engineering. It was held to develop a path to overcome the barriers and challenges identified in *Technology Vision 2020: The Chemical Industry*. *Technology Vision 2020* details the challenges faced by the U.S. chemical industry as it strives to maintain its competitive position into the next millennium. The meeting agenda appears below, and an attendee list is given in Appendix B. The detailed technical barriers and research needs are given in Appendix C. Slides from the presentations given to set the stage for the workshop are given in Appendix E.

Breakout sessions were used in the workshop to allow participants to focus on their technical areas of expertise. Each breakout group was given the broad goal of determining how the technology they were discussing could help in meeting the performance targets for reducing energy and raw materials usage and the generation of wastes as described in Section II. The task of each breakout group was to scope out the technical challenges facing reaction engineering in order for it to be used to meet the workshop indicator goals, identify technical barriers to meeting those challenges, and to list and prioritize the research needed to address the barriers.

The workshop participants were initially asked to identify technical barriers and research needs by evaluating industries which utilize reaction engineering: basic chemicals, specialty chemicals, pharmaceuticals, and polymers. These research needs were then used as the basis for identifying research needs across technical development areas related to reaction engineering: reactor design, chemical mechanisms, catalysis, and novel reactors. Participants sorted the latter prioritized research needs into four broad time frames in which they should be conducted: 0–3 years, 3–10 years, 10+ years, and ongoing.

# Reaction Engineering Workshop

*Renaissance Hotel, Dallas, Texas*
October 30–31, 1999

### *SATURDAY, OCTOBER 30*

8:00 A.M. Breakfast

**8:00–5:00 Vision 2020 Reaction Engineering Workshop**

| | | |
|---|---|---|
| 8:00–8:35 | Welcome | David Klipstein,Workshop Chair |
| 8:35–9:05 | Workshop Expectations | Hank Kenchington, DOE |
| 9:05–9:45 | Current and Future Issues in Reaction Engineering | Lanny Schmidt, University of Minnesota |
| 9:45–10:05 | Workshop Goals and Procedures | David Klipstein |
| 10:05–10:35 | Refreshment Break | |
| 10:35–12:15 | Breakout Sessions by Industry Segment | |
| 12:15–1:30 | Collection and Management of Data (Over Lunch) | Greg McRae, MIT |
| 1:30–4:00 | Breakout Sessions by Industry Segment (Continued) | |
| 4:00–5:00 | Reports from Breakout and Day's Wrap-Up | |

### *SUNDAY, OCTOBER 31*

8:00 A.M. Breakfast

**8:00–5:00 Vision 2020 Reaction Engineering Workshop**

| | | |
|---|---|---|
| 8:30–9:10 | Reaction Engineering 2020, An Academic Perspective | Klavs Jensen, MIT |
| 9:10–9:50 | Reaction Engineering 2020, An Industrial Perspective | Jan Lerou, DuPont |
| 9:50–10:30 | Reaction Engineering in a Process Context | Herman DeMeyer, Bayer |
| 10:30–10:50 | Refreshment Break | |
| 10:50–12:30 | Breakout Sessions by Technology Topic | |
| 12:30–1:30 | Working Lunch | |
| 1:30–2:30 | Breakout Sessions by Technology Topic (Continued) | |
| 2:30–2:50 | Refreshment Break | |
| 2:50–4:15 | Reports from Breakout Sessions and Workshop Wrap-Up | |
| 4:15 | Workshop Adjourns | |

# APPENDIX B
# WORKSHOP PARTICIPANTS

| Name | Affiliation | Industrial Breakout Session | Technical Breakout Session | Workshop Function |
|---|---|---|---|---|
| *Andrews, Art* | *Merck Research Laboratories* | *Pharmaceuticals* | *Mechanism Development* | *Session Chair* |
| *Anthony, Ray* | *Texas A&M University* | *Pharmaceuticals* | *Catalysis* | |
| *Barton, John* | *Oak Ridge National Laboratory* | *Pharmaceuticals* | *Catalysis* | *Scribe* |
| *Chuang, Steven S. C.* | *University of Akron* | *Pharmaceuticals* | *Catalysis* | |
| *Cochran, Hank* | *Oak Ridge National Laboratory* | — | *Mechanism Development* | *Scribe* |
| *Colakyan, Manuk* | *Union Carbide* | *Specialty Chemicals* | *Mechanism Development* | |
| *Coy, Dan* | *Nalco Chemical Company* | *Specialty Chemicals* | *Reactor Design* | |
| *De Meyer, Herman* | *Bayer* | *Specialty Chemicals* | *Novel Reactors* | |
| *DePaoli, David* | *Oak Ridge National Laboratory* | *Specialty Chemicals* | *Reactor Design* | *Scribe* |
| *Dudukovic, Mike* | *Washington University* | *Basic Chemicals* | *Reactor Design* | *Session Chair* |
| *Epling, Bill* | *University of Alabama* | *Basic Chemicals* | *Mechanism Development* | |
| *Frisch, Michael* | *Gaussian* | *Specialty Chemicals* | *Mechanism Development* | |
| *Green, William* | *MIT* | — | *Mechanism Development* | |
| *Gupta, Ramesh* | *Exxon* | *Basic Chemicals* | *Novel Reactors* | |
| *Harold, Mike* | *DuPont* | — | *Catalysis* | |
| *Jensen, Klavs* | *MIT* | — | *Novel Reactors* | |
| *Kenchington, Hank* | *Department of Energy* | *Basic Chemicals* | — | |
| *Klipstein, David* | *Reaction Design* | *Specialty Chemicals* | *Mechanism Development* | *Coordinator* |
| *Koros, Robert M.* | *Exxon Research and Engineering* | *Specialty Chemicals* | *Reactor Design* | *Session Chair* |
| *Krambeck, Fred* | *Mobil* | — | *Reactor Design* | |
| *Leib, Tiby* | *DuPont Company* | *Basic Chemicals* | *Novel Reactors* | |
| *Lerou, Jan J.* | *DuPont Company* | *Polymers* | *Catalysis* | *Session Chair* |
| *Marek, Milor* | *Prague Institute for Technology* | *Polymers* | *Novel Reactors* | |
| *McGuffin, Victoria* | *Michigan State University* | *Pharmaceuticals* | *Mechanism Development* | |
| *McKinnon, Tom* | *Colorado School of Mines* | *Basic Chemicals* | *Mechanism Development* | |
| *McRae, Greg* | *MIT* | *Pharmaceuticals* | *Reactor Design* | *Session Chair* |
| *Neurock, Matthew* | *University of Virginia* | *Polymers* | *Catalysis* | *Session Chair* |

| Name | Affiliation | Industrial Breakout Session | Technical Breakout Session | Workshop Function |
|---|---|---|---|---|
| *Ng, Ka M.* | *University of Massachusetts* | — | *Reactor Design* | |
| *Papavassiliou, Vasilis* | *Praxair* | *Specialty Chemicals* | *Catalysis* | |
| *Peters, Bob* | *Argonne National Laboratory* | *Pharmaceuticals* | *Reactor Design* | |
| *Reklaitis, Rex* | *Purdue University* | *Polymers* | — | |
| *Rice, Steven* | *Sandia National Laboratory* | *Polymers* | *Mechanism Development* | |
| *Robinson, Sharon* | *Oak Ridge National Laboratory* | *Polymers* | — | *Scribe* |
| *Rogers, Jo* | *American Institute of Chemical Engineers* | *Pharmaceuticals* | — | |
| *Rohr, Don* | *General Electric* | *Polymers* | *Reactor Design* | |
| *Schmidt, Lanny* | *University of Minnesota* | *Specialty Chemicals* | *Novel Reactors* | *Session Chair* |
| *Shollenberger, Kim* | *Sandia National Laboratory* | *Polymers* | *Reactor Design* | |
| *Suppes, Galen* | *University of Kansas* | *Basic Chemicals* | *Catalysis* | |
| *Sun, Yongkui* | *Merck & Company, Inc.* | — | *Novel Reactors* | |
| *Takehara, Don* | *Dow Corning Corporation* | *Specialty Chemicals* | *Mechanism Development* | |
| *Thompson, Tyler B.* | *Dow Chemical Company* | *Basic Chemicals* | *Mechanism Development* | |
| *Tiech, Cheryl* | *Rohm & Haas* | *Polymers* | *Reactor Design* | |
| *Toseland, Bernie* | *Air Products & Chemicals* | *Basic Chemicals* | *Reactor Design* | *Session Chair* |
| *Tsouris, Costas* | *Oak Ridge National Laboratory* | *Basic Chemicals* | *Novel Reactors* | *Scribe* |
| *Tsotsis, Theo* | *University of South Carolina* | *Polymers* | *Reactor Design* | |
| *Weaver, Jack* | *American Institute of Chemical Engineers* | *Specialty Chemicals* | — | |
| *Weiner, Steven C.* | *Pacific Northwest National Laboratory* | *Polymers* | — | |
| *West, David* | *Dow Chemical Company* | *Polymers* | *Novel Reactors* | |
| *Westmoreland, Phil* | *University of Massachusetts* | *Specialty Chemicals* | *Mechanism Development* | |
| *Wolfrum, Ed* | *Natural Renewable Energy Laboratory* | *Specialty Chemicals* | *Novel Reactors* | |

# APPENDIX C
# WORKSHOP TECHNICAL BARRIERS AND R&D NEEDS

Each breakout group at the Reaction Engineering Workshop held on October 30–31, 1999, was asked to scope out the technical challenges facing reaction engineering in order for it to be used to meet the workshop indicator goals, identify technical barriers to meeting those challenges, and to list and prioritize the research needed to address the barriers. The workshop participants were initially asked to identify technical barriers and research needs by evaluating industries which utilize reaction engineering: basic chemicals, specialty chemicals, pharmaceuticals, and polymers. These research needs were then used as the basis for identifying research needs across technical development areas related to reaction engineering: reactor design, chemical mechanisms, catalysis, and novel reactors. Participants prioritized the latter research needs into four broad time frames in which they should be conducted: 0–3 years, 3–10 years, 10+ years, and ongoing.

The various experts who identified the research needs assigned each a priority based upon their perceived importance. Key research needs were those that received enough votes from a significant number of experts to score a relative high ***(H)*** or medium ***(M)***. Other needs were ranked low ***(L)*** based on the small number of or no votes received. All barriers and research needs identified during the workshops are recorded in this Appendix. The tables in this Appendix also include items that were cited as research needs during the workshop but were judged to be research-related instead. The high and medium priority research needs are summarized in the body of the report.

**Table C.A.1**
**Technical Barriers for Basic Chemicals**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Fundamental Science and Data | Current Processes | New Technologies | Institutional/Educational |
|---|---|---|---|
| *Lack of experimental verification of models* ***(H)*** | *Characterization capabilities for large commercial reactors are expensive to apply and of limited value* ***(H)*** | *Dependence on simulation of existing systems limits implementation of new systems* ***(L)*** | *Educational limitations* ***(M)***<br>• *Lack of interdisciplinary teaching*<br>• *Inadequate fundamentals (physics/chemistry)* |
| *Lack of ability to measure and predict properties* ***(H)***<br>• *Physical/chemical*<br>• *Kinetic*<br>• *Transport* | *Sensors and controls for large commercial reactors are expensive and of limited capability****(M)*** | *Dealing with impurities* ***(L)***<br>*Lack of novel reactors* ***(L)*** | *High cost to implement new technologies* ***(L)*** |
| *Lack of undersanding of detailed chemistry for new systems* ***(H)*** | *Complex feedstocks result in waste generation and energy usage* ***(M)*** | *High perceived risk (economic and safety)****(M)*** | *Cost of regulatory compliance limits implementation of new technologies* ***(L)*** |
| *Lack of effective models* ***(M)***<br>• *Computing tools*<br>• *Systems approach*<br>• *Computational fluid dynamics of multiphase flow* | *Current processes not geared to recycle* ***(M)*** | | |
| *Poor understanding of catalysis mechanisms* ***(M)*** | *Lack of integration of individual process steps leads to models that are too crude to support model-based control* ***(L)*** | | |
| *Lack of well-characterized experimental reactors* ***(M)*** | | | |

**Table C.A.2**
**Research Needs for Basic Chemicals**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Fundamental Science and Data *(H)* | Model Verification *(H)* | Characterization *(M)* | Educational/Institutional *(M)* |
|---|---|---|---|
| *Need capability to predict properties*<br>• *Kinetics*<br>• *Transport*<br>• *Physical/chemical properties* | *Need new novel reactor systems which can be tested in laboratory* | *Need better characterization capabilities for laboratory- and industrial-scale reactors* | *Need interdisciplinary training* |
| | *Need to use data taken under industrial conditions for model verification* | *Need simpler, cheaper, more robust equipment* | *Need industrial exposure for facility* |
| *Expand molecular modeling capabilities*<br>• *Solutions*<br>• *Functional organic rules* | *Develop systematic method for measurements*<br>• *Standardize techniques*<br>• *Fine-scale CFD modeling* | *Need new techniques for characterization*<br>• *Local flow components*<br>• *Phase fractions for multiphase flows*<br>• *Composition*<br>• *Temperature* | *Need sustainability training* |
| | | | *Need to build teamwork in educational process* |
| | | | *Need ongoing design problems* |
| | *Develop experimental techniques for opaque flows, steel reactors, and large-scale reactors* | | *Increase interaction between modelers and experimentalists* |

**Table C.B.1**
**Technical Barriers for Specialty Chemicals**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Fundamental Science and Data | Processes | Equipment | Institutional/Educational |
|---|---|---|---|
| *Lack of CFD models with reaction and catalysis* ***(H)*** | *Lack of efficient alternatives to large-scale reactors* ***(H)*** | *Lack of effective in-line sensors* ***(H)***<br>*Improved analytical precision*<br>• *Lower cost*<br>• *More robust*<br>• *Faster* | *Sustainability impact on environment* ***(M)*** |
| *Lack of capability to predict product quality and performance a priori* ***(M)***<br>• *Models too imprecise*<br>• *Validation lacking* | *Lack of selectivity* ***(L)***<br>*Lack of efficient methods to design combination reactors and separation systems* ***(L)*** | | *Need multidisciplinary education to handle highly integrated knowledge* ***(M)*** |
| *Inability to predict best reactor process by virtual process optimization* ***(M)*** | | | |
| *Lack of models to predict catalytic effects* ***(M)*** | | | |

**Table C.B.2**
**Research Needs for Specialty Chemicals**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Fundamental Science and Data | Reactor Design | Characterization | Educational/Institutional |
|---|---|---|---|
| *Develop more sophisticated models* ***(H)***<br>• *To predict product properties a priori*<br>• *For reactor/process selection*<br>• *For catalyst reactor design* | *Increase reaction selectivity* ***(H)***<br>• *Biochemistry, enzymes, biomimetics*<br>• *Catalysis, biocatalysis*<br>• *Combinatorial chemistry*<br>*Design efficient reactors* ***(M)***<br>• *Good understanding at small scale*<br>• *Novel reactors* | *Improve on-line effectiveness of chemical sensors* ***(M)***<br>• *Cheap*<br>• *Reliable*<br>• *Nonintrusive* | *More rounded education with up-to-date skills* ***(L)***<br>*Better tools for projecting environmental impact* ***(L)*** |

**Table C.C.1**
**Technical Barriers for Pharmaceuticals**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Fundamental Science and Data | Current Processes | New Technologies | Institutional/Educational |
|---|---|---|---|
| *Lack of synthesis modeling tools for system* ***(H)*** | *Lack of catalysts for specific applications, especially stereospecificity* ***(H)*** | *Lack of cross-disciplinary collaboration, particularly between process chemist and engineer* ***(H)*** | *Simultaneous regulation of the product and the process limits development opportunities* ***(M)*** |
| *Lack of high-speed reaction/ synthesis screening tools* ***(M)*** | *Separations selectivity is often low* ***(M)*** | *Large molecule separations are particularly difficult/ expensive* ***(L)*** | *Tools do not exist for risk and resource management and resource allocation in the discovery process* ***(L)*** |
| *Lack of detailed chemical mechanisms* ***(M)*** | *Bioreactor systems for novel products are rare* ***(M)*** | *Lack of financial incentive to implement the 2020 goals. For example, the pharmaceutical industry will not be impacted by water shortage. Batches tend to be low volume* ***(L)*** | *The discrete nature of unit operations makes it difficult to manage the process as a whole* ***(L)*** |
| *Lack of impurity prediction capability* ***(M)*** | *Bioreactor design methods are too simplistic* ***(L)*** | *Separations and reactions have historically been developed independently. This makes it difficult to optimize them together* ***(L)*** | *The demand for construction of sterile facilities makes production difficult and expensive* ***(L)*** |
| *Lack of data and methods for estimating thermo- physical properties, mechanisms, actions, solvent effects, chiral processing, etc.* ***(L)*** | *Sensors are not durable enough to withstand many process conditions* ***(L)*** | *Lack of technology transfer from other sciences that might be used to improve pharmaceutical reaction engineering* ***(L)*** | *University-level training rarely extends beyond bulk and continuous processing, which means that many engineers are unprepared to work in the pharmaceutical industry* ***(L)*** |
| *Lack of instrumentation and models for probing metabolic pathways* ***(L)*** | *Lack of suitable instumentation for tracking reaction intermediates* ***(L)*** | *Lack of flexible continuous reactor concepts* ***(L)*** | *There is some geographic fragmentation in terms of disseminating information to outsourcing firms that might produce several intermediate products* ***(L)*** |
| *Lack of combinatorial techniques to evaluate synthesis options. A priori design is difficult* ***(L)*** | *Lack of highly selective on-line monitors* ***(L)*** | *Solvents need to be more environmentally benign* ***(L)*** | |
| *Lack of robust scheduling tools for batch processes* ***(L)*** | *Lack of sensor to support model-based control* ***(L)*** | *Pharmaceuticals have shorter and shorter timelines for development* ***(L)*** | |
| *Lack of predictive models and control systems for reactors using immobilized enzymes* ***(L)*** | *Batch processing limits our options for redesigning the reaction* ***(L)*** | *Multiple process optimization (speed, yield, intermediates) is difficult* ***(L)*** | |
| *Lack of fundamental understanding regarding usage of surface assembled coatings (e.g., chromatographic polymers)* ***(L)*** | *Chromatography techniques/ processes do not scale up well* ***(L)*** | | |
| | *Lack of genetic tools for micro and molecular biologists to generate and control gene cloning* ***(L)*** | | |
| | *Lack of inexpensive, safe, effective sterilization systems* ***(L)*** | | |

**Table C.C.2**
**Research Needs for Pharmaceuticals**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Discovery Stage | Product Synthesis | Process Development | Plant Operations |
|---|---|---|---|
| *Develop better product screening techniques* ***(H)*** | *Develop more selective catalysts* ***(H)*** | *Design improved reactor systems* ***(H)*** | *Develop robust scheduling tools for batch processes* ***(M)*** |
| *Develop better combinatorial techniques to evaluate synthesis options* ***(H)*** | *Determine thermochemistry and properties data* ***(H)*** | • *High purity, easily separated product*<br>• *High selectivity*<br>• *High yield* | *Develop highly specific durable, online instrumentation* ***(M)*** |
| *Improve experimental design to reduce cost and time requirements* ***(H)*** | • *Chiral compounds*<br>• *Isomers*<br>• *Nucleation/crystallization* | *Reduce time and cost for process development* ***(H)*** | *Develop cheap, easily implemented sterilization processes* ***(M)*** |
| *Develop fundamental-based models for synthesis chemistry and entire system* ***(M)*** | *Develop highly specific, durable, online instrumentation* ***(M)*** | • *Revamp registration process*<br>• *Cross-disciplinary training*<br>• *Better resource management tools*<br>• *Model development cycle to manage personnel and risk* | |
| | *Understand solvation effects* ***(M)*** | *Integrate solvation effects into synthesis models* ***(M)*** | |

**Table C.D.1**
**Technical Barriers for Polymers**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Materials | Processes | Feedstock | Institutional/Educational |
|---|---|---|---|
| *Lack of computational tools to design polymers and catalysts* ***(H)*** | *Lack capability to determine effect of reactor operations on final product properties* ***(H)*** | *Lack of ability to make polymers from gas and agricultural feedstocks* ***(M)*** | *Time frame from development to market is too long using current methods* ***(L)*** |
| *Lack of clearly defined relationships between properties, structure, and performance* ***(H)*** | • *Connect product properties to process variables*<br>• *Understand effect of dynamic/ transient properties on polymer structure* | *Lack of ability to use $CO_2$ and water as polymer raw materials* ***(L)*** | |
| *No good processes to depolymerize polymers* ***(M)*** | *Lack of computational tools for modeling polymerization chemistry* ***(H)*** | | |
| *Lack of design capabilities to produce smart, multifunctional materials* ***(L)*** | *Lack of understanding of which processes determine polymer microstructure* ***(H)*** | | |
| *Lack of high-activity, selective catalysts* ***(L)*** | *Lack of data to validate polymerization models* ***(M)*** | | |
| *Lack of well defined material substitution requirements* ***(L)*** | *Lack of detailed understanding of combined step processes* ***(M)*** | | |
| *Lack of data to validate polymerization models* ***(L)*** | • *RM*<br>• *Reactive extrusion*<br>• *Reactive formation/ separations* | | |
| *Lack of fundamental understanding of complicated large molecule chemistry* ***(L)*** | *Lack of efficient ways to produce polymers* ***(L)*** | | |
| *Lack of understanding of 3–5 monomer copolymerization* ***(L)*** | *Lack of tools to control spatiotemporal gradient patterns in reactors* ***(L)*** | | |
| *Poor access to material substitution requirements from other industries* ***(L)*** | *Lack of advanced monitors and controls* ***(L)*** | | |
| | *No well developed technology for solventless processes* ***(L)*** | | |
| | *Lack of methodology for meeting more strict quality control requirements* ***(L)*** | | |
| | *Empirical screening methods are inadequate* ***(L)*** | | |

**Table C.D.2**
**Research Needs for Polymers**
*(H = High Priority, M = Medium Priority, L = Low Priority)*

| Modeling | Materials Development | Processing |
|---|---|---|
| *Develop advanced combinatorial methods for polymer property screening* ***(H)*** | *Design new recyclable polymers* ***(H)*** | *Understand impact of process conditions on polymer product properties* ***(H)*** |
| *Develop more accurate property prediction capabilities* ***(H)***<br>• *Infrared*<br>• *Materials strength* | *Design processes to disassemble existing polymers for recycle* ***(H)***<br><br>*Need to couple product and process development methods* ***(L)*** | • *Link micro-scale to meso-scale to macro-scale properties*<br>• *Understand of interaction between properties, structure, and performance*<br>• *Understand catalyst and polymer design* |
| *Develop reactive CFD models for large molecules polymer systems* ***(M)*** | *Need course to fine hierarchy of models to speed development* ***(L)*** | *Need online monitors for in situ property measurement and reactor analysis* ***(M)*** |
| *Need models to identify and control spatio-temporal gradient patterns in reactors* ***(M)*** | | *Develop novel ways to combine reactions and separations* ***(M)*** |
| *Link materials properties with process models* ***(L)*** | | *Develop design methodology for single step processes which combine reaction, heat transfer, and separations* |
| *Develop bench and plant capability to validate models* ***(L)*** | | *Develop online model-based control strategies* ***(L)*** |
| *Develop modeling algorithms to deal with multiscale approaches* ***(L)*** | | *Develop methodology to identify and control spatial gradients in reactors* |
| *Identify accurate semiempirical parameters and methods for generating inputs to models* ***(L)*** | | |

**Table C.E.1**
**Research Needs for Reactor Design and Scale-Up**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Need Category | All (Ongoing Processes) | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Fundamental Data and Science*** | *Data for validation of models across multiple scales* ***(H)***<br><br>*Capture uncertainty variability in measurements of data used in models* ***(H)*** | *Obtain better characterization of lab-scale reactors for obtaining kinetic data* ***(H)***<br><br>*Obtain thermochemical and transport property data for complex systems such as chiral isomers* ***(H)*** | *Develop laboratory reactors for synthesis of specific complex chemistries* ***(H)***<br><br>*Obtain thermochemical and transport property data for complex systems such as chiral isomers* ***(H)*** | *Develop micro-reactors for obtaining experimental design and modeling data* ***(H)*** |
| ***Experimental Tools*** | | | *Develop accelerated methods to predict catalysts deactivation and time-dependent product properties* ***(M)*** | *Develop methodology to accelerate the scale-up of processes including redefining the role of pilot scale* ***(M)*** |
| ***Processing*** | *Develop methodology for* ***(H)***<br>• *Scheduling optimization*<br>• *Parameter estimation*<br>• *Application of experimental design*<br>• *Risk/resource management*<br><br>*Develop improved process sensors* ***(M)***<br>• *Fast, cheap, reliable* | *Improved sensors* ***(M)***<br>• *Advanced instrumentation strategies for tracking progress of reactions* | *Improved sensors* ***(M)***<br>• *Advanced instrumentation strategies*<br>• *Smart tracers for in-situ, real-time measurement of composition, temperature, flow, pressure, and telemetry* | *Improved sensors to support model-based control* ***(M)*** |
| ***Modeling*** | *Modeling for safety, environmental, and quality assessment* ***(L)***<br><br>*Develop methods for assessing information value* ***(L)***<br>• *Sensibility/uncertainty*<br>• *Model analysis*<br>• *Analysis to drive investments*<br>• *Verification* | *Develop models to combine reactions and transport* ***(H)***<br>• *Scaling tools*<br>• *Property prediction*<br><br>*Develop reactor synthesis models* ***(H)***<br>• *Geometry*<br>• *Heat & mass transfer*<br>• *Materials*<br>• *Selectivity*<br>• *Trace products*<br>• *Separations ease* | *Integrate component models to allow total system modeling and optimization* ***(H)*** | |
| ***Education*** | *Develop improved educational tools* ***(L)***<br>• *Cross-disciplinary training*<br>• *Closer ties with industry*<br>• *Fellowships from industry* | | | |

**Table C.F.1**
**Research Needs for Chemical Mechanisms**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Need Category | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|
| ***Experimental Tools*** | *Develop accessible microkinetic experimental capabilities* ***(H)***<br>• *Heterogeneous catalysis*<br>• *Multiphase systems* | *Better sensors to track progress of reactions* ***(M)***<br>• *Fast response*<br>• *Online analyses*<br>• *Trace species*<br>• *Multiphase* | |
| ***Mechanism Capabilities*** | *Improve precision and ease of application of quantum chemistry methods for calculating kinetic and thermodynamic properties* ***(M)*** | *Develop methods to integrate solvent effects into reaction models* ***(H)***<br>• *Especially for weak forces*<br>*Expand mechanism development methods* ***(M)***<br>• *Electrochemical processes*<br>• *Photon processes*<br>• *Plasma-driven processes*<br>*Develop better understanding of chiral reactions & separations* ***(L)*** | |
| ***Mechanism Inputs*** | *Develop models with surface species under full range of process conditions* ***(M)***<br>*Obtain thermophysical, thermochemical, and kinetic data for properties models* ***(M)*** | *Obtain thermophysical, thermo-chemical, and kinetic data for properties models* ***(M)*** | *Develop theoretical and experimental methods for macroscopic properties from molecular structures* ***(H)*** |
| ***Mechanism Development Tools*** | *Develop commerical grade automatic mechanism reduction tools* ***(L)***<br>*Couple process chemistry models with experiment to elucidate understanding* ***(M)*** | *Develop practical tools which couple process chemistry with process modeling* ***(H)***<br>• *Better use interface*<br>• *Better software integration*<br>• *More robust numerics* | *Develop mechanisms with capability to predict full range of significant species* ***(L)***<br>*Develop better means of discriminating mechanisms* ***(L)*** |

**Table C.G.1**
**Research Needs for Catalysis**
*(H = High Priority, M = Medium Priority, L = Low Priority)*

| Need Category | All (Ongoing Processes) | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Funda-mental Data and Science*** | *Fischer-Tropsch synthesis* ***(M)***<br>*Mechanistic studies* ***(M)***<br>*Catalysis of alternative feedstocks* ***(M)***<br>*Biocatalized polymerization* ***(M)***<br>*By-product & waste minimization* ***(L)***<br>*Synthesis of catalysts with specific site architectures* ***(L)***<br>*"One pot" syntheses* ***(L)***<br>*Electrochemcal catalysis* ***(L)***<br>*Bond-specific catalysts (typically biological)* ***(L)*** | *Phase-transfer catalysts* ***(L)*** | *Fuel-cell-related catalysis* ***(H)***<br>*Stereoselective synthesis* ***(H)***<br>*Selective oxidation catalysts****(M)***<br>*Catalyst support design* ***(M)***<br>*Functional olefin polymerization* ***(L)***<br>*Define potential alkylation catalysis routes* ***(L)*** | *Hydrocarbon activation* ***(M)***<br>*Understanding and predicting transport occurring in heterogeneous systems* ***(L)*** |
| ***Experi-mental Tools*** | *Development techniques for high throughput screening and synthesis* ***(M)***<br>*Tomographic, MRI, or other visualization techniques for catalyst characterization.* ***(L)***<br>*Field-enhanced processes* ***(L)*** | *Microreactors for studying nano-contact issues* ***(L)*** | *Better in situ techniques for tracking and characterizing catalyst performance* ***(H)***<br>*Lab bench reactors that more closely mimic industrial conditions* ***(L)*** | *Detection of transient intermediates (tightened temporal analysis of the reaction, highly specific to the intermediates which form, etc.)* ***(M)*** |
| ***Processing*** | *Easily recoverable, process-friendly, nontoxic, homogeneous catalysts* ***(L)***<br>*High throughput process screening tools* ***(L)***<br>*Influence on intrinsic kinetics from extrinsic environment* ***(L)*** | *Advanced analysis tools and precise data screening (e.g. neural nets)* ***(M)***<br>*Retrofitting existing reactors with new catalysts* ***(L)*** | *System integration (laboratory): combining experimental tools and modeling tools to give kinetics and reactor design in one easy step.* ***(M)***<br>*Model-based control of catalytic processes****(L)***<br>*Develop catalysts that are more resistant to deactivation and aging* ***(L)*** | *System integration (plant scale): analyzing and optimizing both the catalyst and reactor at the same time* ***(H)***<br>*Extracting fundamental understanding from plant scale processes/data* ***(M)***<br>*Develop catalysts with improved ability to adapt to changing feedstock* ***(L)*** |
| ***Modeling*** | *Build models that*<br>• *Are based on fundamentals rather than empirical* ***(M)***<br>• *For transport* ***(M)***<br>• *Can predict catalyst life* ***(M)***<br>• *Can predict physical/chemical properties* ***(L)*** | *Build models that will accelerate development for new catalysts (i.e. design a catalyst prior to applying a combinatorial technique to find out how it works best. High input screening would then become much more intelligent.)* ***(M)*** | *Develop reactive CFD software to model catalyst performance* ***(M)***<br>*More rigorous prediction of product quality and performance a priori (model and validation)* ***(M)***<br>*Heterogeneous catalyst tools* ***(L)***<br>*Better reactor design from minimal data* ***(L)*** | *Develop computational tools for catalyst design to produce materials with desired properties* ***(M)***<br>*Catalyst design through combined experimental and mechanistic understanding and computational chemistry* ***(L)*** |

*(continued on the next page)*

**Table C.G.1**
**Research Needs for Catalysis (*continued*)**

| Need Category | All (Ongoing Processes) | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Design*** | *Develop catalyst designs that are* ***(M)***<br>• *More resistant to attrition, coking, and deactivation*<br>• *Able to focus on specific bond sites*<br>*Develop new screening tools for selectivity****(L)***<br>*Develop methodology to accelerate catalyst development processes* ***(L)*** | *Develop techniques for improving contacting patterns between catalyst and reactor* ***(M)*** | *Supercritical and subcritical catalysis* ***(M)***<br>*Micellar catalysis* ***(L)***<br>*Need increased selectivity for site-specific catalysts, biocatalysts, enzymes, biomimetics* ***(M)*** | *Design of catalysts for applications involving solid matrices (e.g., coal, complex matrix polymers)* ***(H)*** |
| ***Education*** | | *Industry experience for faculty* ***(L)***<br>*Interdisciplinary team projects* ***(L)*** | *Cross-disciplinary training, education and thought processes* ***(M)***<br>*Incentives and resources for development of interdisciplinary courses* ***(L)*** | |

**Table C.H.1**
**Research Needs for Novel Reactors**
(H = High Priority, M = Medium Priority, L = Low Priority)

| Need Category | All (Ongoing Processes) | Near Term (0–3 Years) | Mid-Term (3–10 Years) | Long-Term (10+ Years) |
|---|---|---|---|---|
| ***Fundamental Data and Science*** | *Develop techniques to estimate microproperties and phenomena* ***(M)***<br>*Develop improved methodology for exploiting external field-assisted reactions* ***(H)*** | | *Develop automated synthesis* ***(M)*** | *Develop reactors to produce artificial cells* ***(M)*** |
| ***Materials*** | *Develop better materials for* ***(H)***<br>• *Extreme conditions*<br>• *Micro-fabrication*<br>• *Catalysts*<br>• *Sensors* | | | |
| ***Design*** | *Improve systems intergration* ***(H)***<br>*Develop multiscale design capabilities* ***(H)***<br>*Develop self-assembling reactors* ***(H)***<br>*Develop intensified reactors* ***(H)***<br>*Develop structured contacting* ***(H)***<br>*Develop biomolecular design capabilities* ***(H)***<br>*Develop rapid heating/ cooling systems* ***(H)*** | *Develop ultra-low cost reactors* ***(M)*** | *Develop optimized fuel processors* ***(M)*** | |
| ***Demonstrate Value*** | | *Develop/demo improved photochemical reactors* ***(H)***<br>*Develop/demo immobilized cell & enzyme reactors* ***(H)***<br>*Develop more cost effective reactors for extreme conditions* ***(M)*** | *Develop/demo electrochemical reactors* ***(H)*** | *Develop/demo biomimetic reactors* ***(H)*** |

# APPENDIX D
# CHEMICAL INDUSTRY STATISTICS

**Industry Overview:** The U.S. chemical industry products include industrial gases, large-volume commodity chemicals and polymers, chemical products for agricultural and medicinal uses, and performance-targeted chemical and polymer specialties. The chemical industry obtains raw materials from the petroleum refining, natural gas, and mining industries, as well as from biological sources. The United States is the world's largest producer of chemicals. Countries that rank next in total production are Japan, Germany, and France. In terms of exports, Germany is the global leader. The United States ranks second, with approximately 14 % of total exports worldwide. The chemical industry is the largest exporting industry in the U.S. economy. The U.S. chemical industry runs one of the largest trade surpluses of any industry sector, and it ranks as the largest manufacturing sector in terms of value added. Overall, the chemical industry is the third largest manufacturing sector in the nation.

The U.S. chemical industry

- accounts for about 24% of the world's total chemical output
- produces 1.9% of U.S. GDP and 11% of all U.S. manufacturing; total shipments reached $372 billion in 1996
- includes 12,000 plants producing 70,000 chemicals; 95% produced in 2,000 batch facilities
- includes 170 U.S. companies with more than 2,800 facilities abroad; 1,700 foreign subsidiaries or affiliates operating in the United States.
- exported $62 billion and imported $45 billion in 1996; 29% of international trade is intra-company; over 25% of trade with Canada and Mexico
- accounts for $1 of every $10 of U.S. goods exported
- employs over a million people in the United States, 58% are production workers who earn one-third more than the U.S. manufacturing average
- concentrates 63% of production in 10 states: TX, NJ, LA, IL, NC, CA, OH, PA, NY, SC; 70% of primary petrochemicals produced in Texas and Louisiana
- invested over $34 billion on new plants and equipment in 1996
- values energy costs at only 9% of industry shipments
- value added $126 billion in 1994
- income after taxes rose to $45 billion and shareholder's equity increased to 22.6% in 1996

Many view the chemical industry as the "keystone" manufacturing industry. This is because the preponderance of its products are inputs to other manufacturing industries as well as agriculture and mining. Of the 70,000 products produced by the chemical industry, the majority are feedstocks that improve the productivity and quality of goods manufactured by other industries:

- basic chemicals—e.g., acids, alkalies, salts, and organic chemicals
- chemical products used in further manufacture (intermediates)—e.g., synthetic fibers, plastic materials, and color pigments
- finished chemical products used for ultimate consumption—e.g., paints, fertilizers, and explosives

In 1994, the industry produced goods valued at $341.3 billion with $82.9 billion for intraindustry shipments and $258.4 in final shipments. The final shipments consisted of ($ billion):

- rubber and plastics products $28.5
- home furnishings, textiles, and apparel $19.6
- petroleum refining $7.0
- paper and allied products $7.2
- electrical and electronic equipment $7.2
- machinery and instruments $4.8
- all other manufacturing $23.1
- motor vehicles $2.9
- primary metals $5.2
- agriculture $12.6
- mining $1.9
- construction $9.8
- exports $49.0
- healthcare and education $28.0
- consumers $44.6
- services and other $9.3

**R&D in the Chemical Industry:** A major factor in the long-term success of the industry has been its traditionally large R&D program. It

- is one of the eight most research-intensive U.S. industries
- employees 100,000 scientists, engineers, and technicians in chemical-related R&D
- receives about one out of every eight U.S. patents
- invested over $18.3 billion on R&D in 1996
- is led by pharmaceuticals R&D which accounts for more than one-half (57%) of the chemical industry's R&D spending

**Energy Usage by the Chemical Industry:** The chemical industry is the second largest energy-consuming industry in the United States. In 1994, it consumed about 7 percent of the total energy consumed in the United States. The chemical industry used 25% of the estimated manufacturing energy used by industry in 1994. Overall, four segments of the chemical industry—inorganic chemicals, organic chemicals, plastics, and fertilizers—consumed about 85% of all fuel and electricity used in the chemical industry in 1994. Industry statistics include:

- total energy needs equivalent to 2.8 million barrels of crude oil per day: natural gas, 42%; crude oil and derivatives, 41%; electricity, 9%; coal, 4%; others, 4%
- consumed 5.95 quads for feedstocks (2.99) and fuel/power (2.96) in 1996
- Fuel/power costs as a fraction of production costs are quite variable: e.g., high for industrial gases (40–50%), lower for industrial organics chemicals (less than 10%)
- energy consumption by product area (in quads): organics, 2.6; inorganics, 0.7; plastics, 0.9; agri-chemicals, 0.7
- energy costs in the industrial gas segments of the industry account for 40–50% of total operating costs
- overall efficiency of energy used in the chemical industry improved by over 40% between 1974 and 1996
- the proportion of energy used for feedstocks grew from 39% in 1970 to 48% in 1996, primarily due to growth of the plastics business
- uses labor less intensively than other manufacturing industries (production workers are 58% of total employment vs. 69% for all manufacturing)

**Environmental Impact of the Chemical Industry:** The chemical industry generates about 2 billion tons of waste per year. The majority is wastewater (91% in 1989) from the industry's manufacturing processes. Air emissions per year are approximately 4.3 million metric tons. The concern about the role greenhouse gases play in the changing character of our climate has focused largely on carbon dioxide, which makes up about 55% of these emissions. Of the total carbon emissions in the United States, the chemical industry contributed 3%. Industry statistics include:

- has regulatory costs growing faster than any other component of most capital budgets
- industry spends more than any other U.S. industry for pollution abatement and control—$7.1 billion in 1994
- total pollution abatement control costs for chemical companies of $14.3 billion slightly exceeded the whole industry's $14.2 billion total after-tax profits for 1989–1993
- pollution abatement by product area in 1994: organics, $919M; inorganics, $159M; plastics, $465M; agri-chemicals, $99 M
- decreased toxic emissions as defined by EPA's Toxic Release Inventory Reporting Program 61% between 1988-1994, while production rose 18%
- 1994 annual emissions (in millions of metric tons): $SO_2$, 0.5; $NO_x$, 0.3; VOC, 1.6; CO, 2.2; particulates, 0.1; lead, 0.0001
- total U.S. greenhouse gas contributions in the 1990s (all sources); $CO_2$, 84%; $CH_4$, 11%; $NO_x$, 3%; chlorofluorocarbons, 2%
- total U.S. carbon emissions 1.45 billion metric tons (1996); by fuel type: oil, 42.1%; coal, 35.5%; natural gas, 22.4%
- total U.S. carbon emissions by industrial sector: electric utilities, 35.6%; transportation, 32.8%; residential, 6.9%; commerical, 4.2%; chemical industry, 2.6%; other industry, 17.9%

**Chemical Industry Vision for 2020:** In 1994, technical and business leaders in the chemical industry began to study the factors affecting the competitiveness of their industry and its rapidly changing business environment. They focused on identifying the common technology challenges that will face the industry over the next 25 years. In the spring of 1996, the industry's sponsoring organizations approved *The Technology Vision 2020: Report of the U.S. Chemical Industry*. The report, "a call to action, innovation, and change," concludes that the growth and competitive advantages of the chemical industry depend on individual and collaborative efforts of industry, government, and academia to improve the nation's R&D enterprise. The *Vision 2020* report identifies four targeted areas:

- New chemical science and engineering technology
- Supply-chain management

- Information systems
- Manufacturing operations

The New Chemical Science and Engineering Technology area is made up of three subareas in chemical science (chemical synthesis, bioprocesses and biotechnology, and materials technology) and three areas of enabling technology (process science and engineering technology, chemical measurement, and computational technologies). Each area and/or subarea are described briefly below:

- *Chemical Synthesis* emphasizes developing new catalysts and reaction systems to prepare economical and environmental safe processes with lowest life-cycle costs.
- *Bioprocesses and Biotechnology* emphasizes improving performance of biocatalysts and improving biochemical processing.
- *Materials Technology* includes enhanced performance in materials, including materials for separation processes, and membranes for chemical processing, packaging, medical, and other separation applications.
- *Process Science and Engineering Technology* emphasizes the development of appropriate design principles, tools, systems, and infrastructures to accommodate a variety of improvements to meet current and emerging needs, including (1) integration of reaction and separation systems such as reactive distillation, membrane reactors, and supercritical fluid systems; (2) production of reactors for new emerging process chemistries; (3) production of existing and new products that reduce significant overall waste, optimize costs, and minimize environmental impact; and (4) development of disassembly procedures for recovery and reuse of materials.
- *Chemical Measurement* emphasizes robust measurement techniques for real-time, highly reliable analyses in practical environments.
- *Computational Technologies* emphasizes that, in order for scientists and engineers to better model more complex fluid dynamics, programs can be developed to incorporate emerging advances in physical models and property databases to provide a readily adaptable architecture.
- *Supply-Chain Management* needs and challenges include market globalization; growth of free trade; regulatory restrictions; transportation; information processing; and environmental, health, and safety concerns.
- *Information Systems* needs and challenges include improvements in networking, communications, and data exchange; improvements; improvements in hardware and software; and changes in policy.
- *Manufacturing and Operations* needs and challenges include equipment and monitoring, process control, process modeling, advisory systems, hardware and software, and open systems and integrated applications.

The status of Vision 2020 implementation can be found on the Web at www.chemicalvision2020.org.

# APPENDIX E
# WORKSHOP PRESENTATIONS

## Welcome, by David Klipstein

### Welcome

- Reaction Engineering Workshop
- Chemical Industry Vision 2020 Project
- Sponsored by
  - DOE Industrial Technology Section
  - Dow Chemical
  - Merck & Co

Reaction Engineering Workshop

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### Saturday Schedule

- 8:30 **Welcome** David Klipstein
- 8:35 **2020,OIT and The Future Needs of Industry** Hank Kenchington, DOE
- 9:05 **Issues in Reaction Engineering** Lanny Schmidt, U of Minnesota
- 9:45 **Workshop Goals and Procedures** David Klipstein
- 10:05 **Refreshment Break**
- 10:35 **Breakout Sessions by Industry Segment**
- 12:15 **Management of Reaction Engineering Data** Greg McRae, MIT (Over Lunch)
- 1:30 **Breakout Sessions by Industry Segment**
- 4:00 **Breakout Reports and Day's Wrap-Up**

Reaction Engineering Workshop

2

### Outline

- Organize by Technology Breakout Topics
- For Each Topic
  - Current State
  - Future State
  - Barriers
  - Research Needs
- Define & Describe Crosscutting Needs as Above

Reaction Engineering Workshop

3

### Goals

- Performance (30%reduction per unit produced)
  - Raw Material Useage
  - Water Useage
  - Energy Useage
  - Toxic Emissions
  - Pollutant Emissions
- Economic
  - Return on Investment (e.g.reactor size, throughput)
  - Development Time & Cost

Reaction Engineering Workshop

4

## Breakout Procedure

- Identify Opportunities
- Define Barriers
- Define Research Needs
- Ballpark Cost/Benefits Impact
- Rank by Cost/Benefit Impact (1-4)
- Define Time Frame
- Sort by Timeframe (S, M, L)
- Report Top Seven with Description (1-2 Lines)
- Add Cross Cuts as Above

Reaction Engineering Workshop

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## Guidelines

- Start with Brainstorm Approach (Hour 1)
  - Accumulate ideas , no screening
- Develop ideas and select best candidates (Hrs 2-3)
- Test and refine best candidates (Hour 4)

The Task

To Identify Opportunities NOT to Detail Projects

Reaction Engineering Workshop

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## Timetable

| | |
|---|---|
| Workshop | October 30-31 |
| Notes Consolidated | October 31- November 5 |
| First Roadmap Draft | February 1 |
| Final Document Ready | August 1 |
| Publication | September 1 |

Reaction Engineering Workshop

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## Sunday Schedule

- 8:30 **Sunday Schedule** David Klipstein
- 8:35 **RE - 2020, An Academic Perspective** Klavs Jensen, MIT
- 9:15 **RE - 2020, An Industrial Perspective** Jan Lerou, duPont
- 9:55 **Reaction Engineering in a Process Context** Herman DeMeyer, Bayer
- 10:35 **Refreshment Break**
- 10:55 **Breakout Sessions by Technology Segment**
- 12:30 **Working Lunch**
- 2:15 **Breakout Reports and Day's Wrap-Up**
- 4:15 **Adjourn**

Reaction Engineering Workshop

8

# Workshop Expectations, by Hank Kenchington

1

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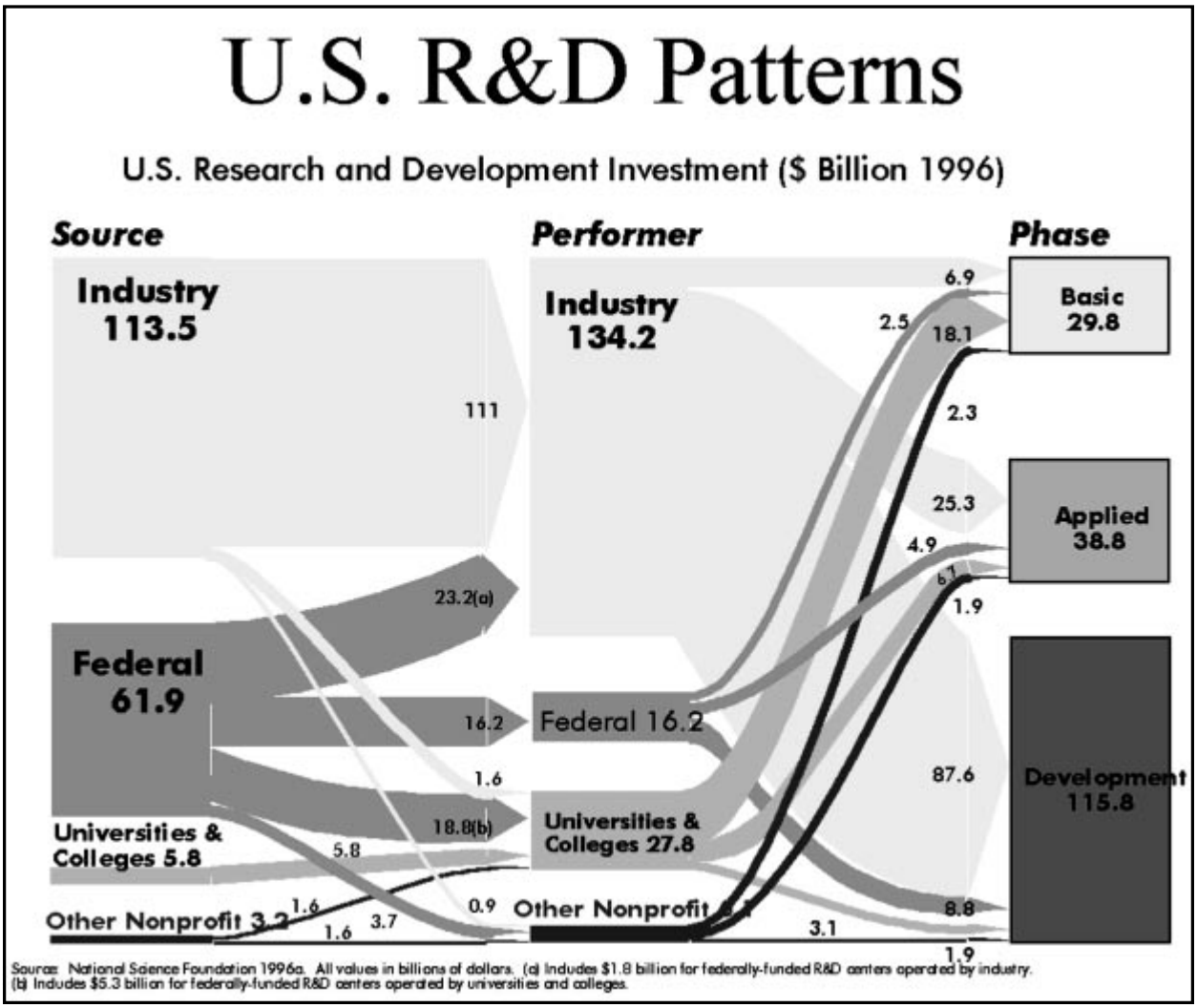


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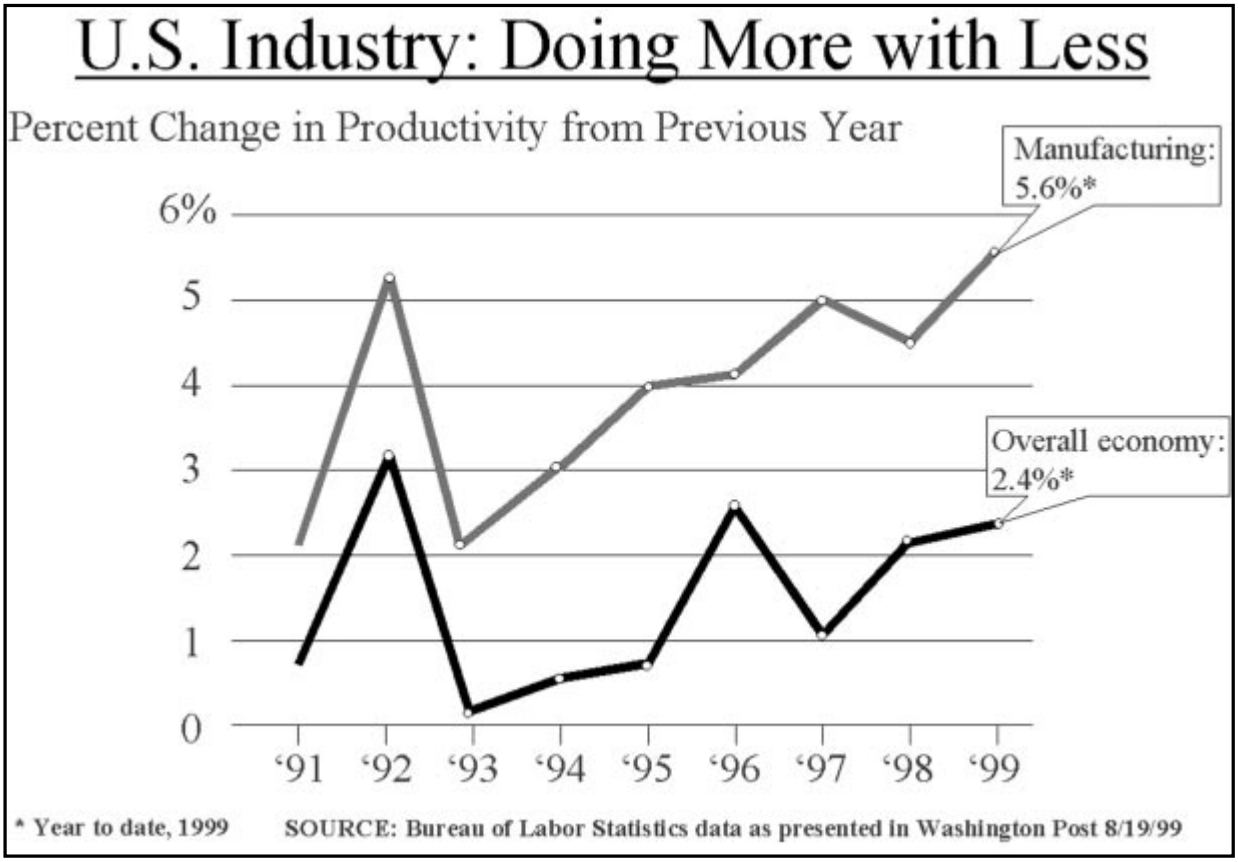


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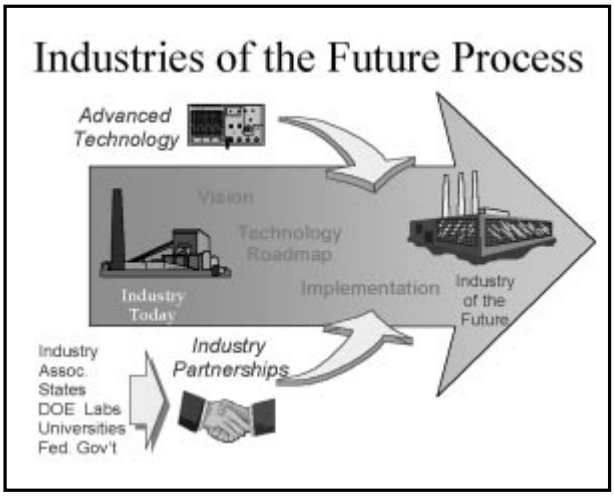
"You need only one competence for the future: *innovation* and the ability to measure performance"

Peter Drucker

in Innovation Strategy for the Knowledge Economy, 1997

5


Industries of the Future Process
Advanced Technology
Vision
Technology Roadmap
Industry Today
Implementation
Industry of the Future
Industry Partnerships
Industry Assoc.
States
DOE Labs
Universities
Fed. Gov't

6

Technology Vision 2020
The U.S. chemical industry...
• Leads the world in technology development, manufacturing, and profitability
• Responsible for R&D breakthroughs that enhance the quality of life
• Leads the world in creating innovative process and product technologies
• Sets the world standard for manufacturing operations that protect worker health and safety
• Is a responsible neighbor who protects environmental quality
• Sets manufacturing standards in energy and raw material efficiency
• Works with academia and government to develop innovative technologies
• Promotes sustainable development
• Chemical Manufacturers Assoc.
• AIChE
• American Chemical Society
• Council for Chemical Research
• SOCMA

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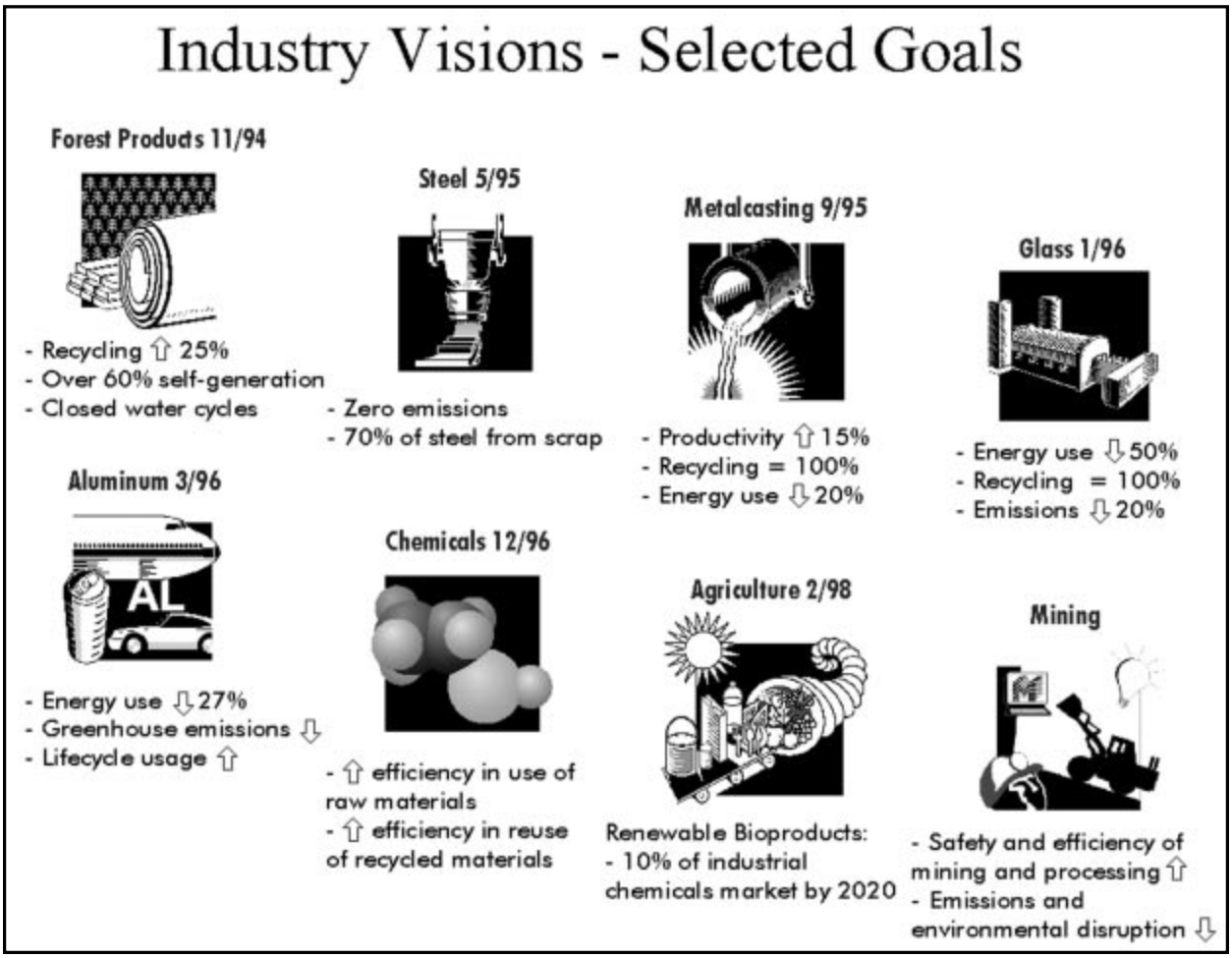
Industry Visions - Selected Goals
Forest Products 11/94
- Recycling ⇧ 25%
- Over 60% self-generation
- Closed water cycles
Steel 5/95
- Zero emissions
- 70% of steel from scrap
Metalcasting 9/95
- Productivity ⇧ 15%
- Recycling = 100%
- Energy use ⇩ 20%
Glass 1/96
- Energy use ⇩ 50%
- Recycling = 100%
- Emissions ⇩ 20%
Aluminum 3/96
AL
- Energy use ⇩ 27%
- Greenhouse emissions ⇩
- Lifecycle usage ⇧
Chemicals 12/96
- ⇧ efficiency in use of raw materials
- ⇧ efficiency in reuse of recycled materials
Agriculture 2/98
Renewable Bioproducts:
- 10% of industrial chemicals market by 2020
Mining
- Safety and efficiency of mining and processing ⇧
- Emissions and environmental disruption ⇩

7

## Vision 2020: Critical Needs

- New Chemical Science & Engineering Technology
  - –Three Areas of Chemical Science
    - Chemical Synthesis
    - Bioprocesses & Biotechnology
    - Materials Technology
  - –Enabling Technologies
    - Process Science & Engineering Technology
    - Chemical Measurement
    - Computational Technologies
- Supply Chain Management
- Information Systems
- Manufacturing & Operations

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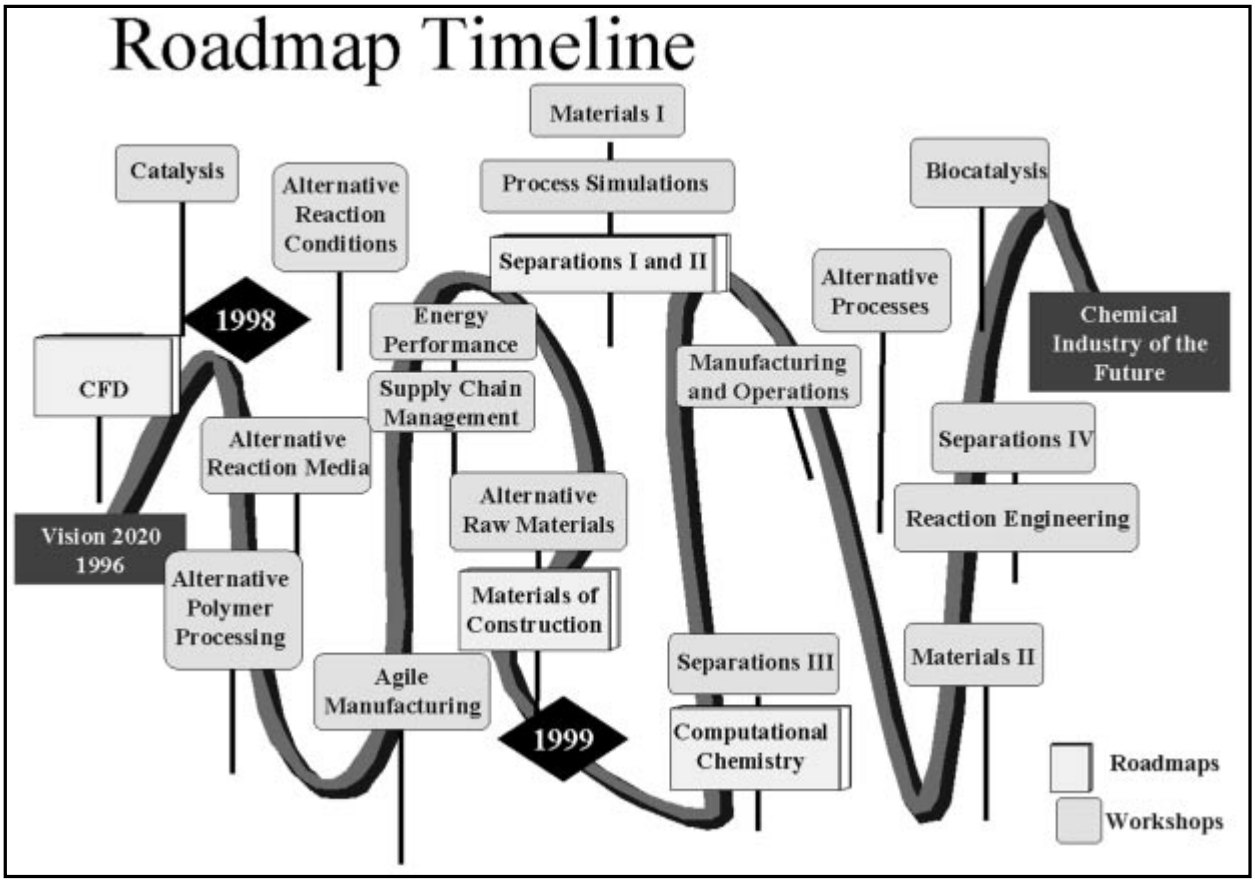


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# Vision 2020 Roadmap Goals

| Roadmap | Lead | Key Goals for 2020 |
|---|---|---|
| Computational Fluid Dynamics | Council for Chemical Research (CCR) | • Shorten lead times to 3-5 years<br>• Shorten plant down times by 50-75%<br>• Improve separation efficiency by 20% |
| Catalysis | BF Goodrich, Sandia, CCR | • Accelerate catalyst discovery process<br>• Develop catalysts with ~100% selectivity |
| Computational Chemistry | Council for Chemical Research | • Increase speed of performance by $2^{10}$<br>– Quantum scale<br>– Atomistic scale<br>– Meso scale |
| Separations | AIChE/CWRT | • 30% reduction in sustainability indicators by 2020 |
| Materials of Construction | Materials Technology Institute (MTI) | • Cut energy use by 30% by 2020<br>• Increasing uptime & yield by 20%<br>• No fugitive emissions |
| Materials Technology | MTI | • Reduce non-reusable materials by 20%<br>• Reduce $CO_2$ emissions per kWh by 30% |
| Alternative Synthetic Pathways | American Chemical Society | • Reduce Btu/$GDP by 20-50%<br>• Reduce separations energy use by 5-50% |

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# Sustainability Indicators

30% Reduction

*Vision 2020*
*1998*
*Separations*
*Roadmap*

**Materials**

$$\frac{\text{Mass of Material Purchased - Mass of Product}}{\text{Value Added}}$$

**Water Consumption**

$$\frac{\text{Volume of Fresh Water Used}}{\text{Value Added}}$$

**Energy**

$$\frac{\text{Net Energy Used (mega-joules)}}{\text{Value Added}}$$

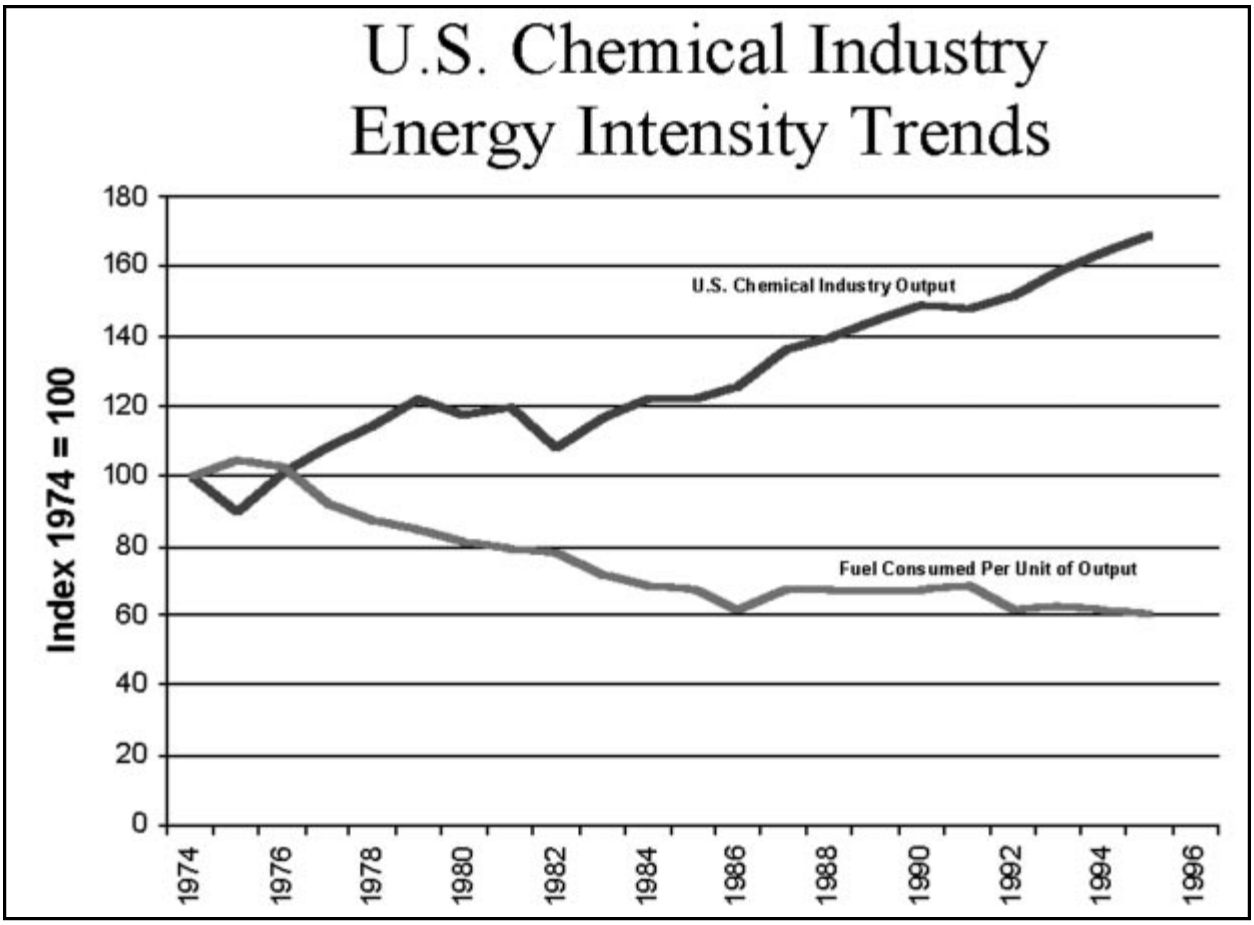
**Pollutant Dispersion**

$$\frac{\text{Total Mass of Recognized Pollutants Released}}{\text{Value Added}}$$

**Toxic Dispersion**

$$\frac{\text{Total Mass of Recognized Toxic Materials Released}}{\text{Value Added}}$$

12

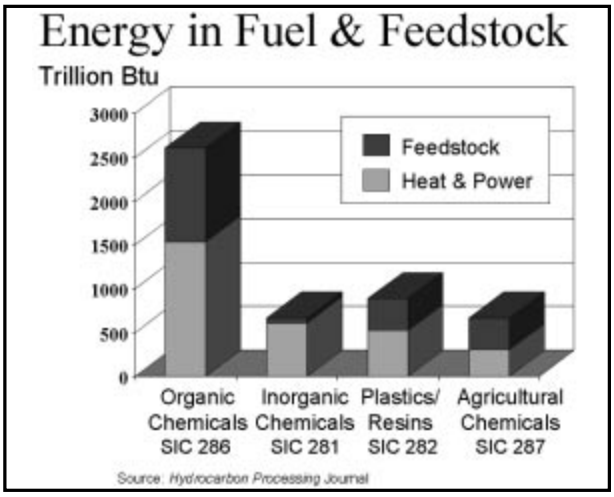



## Significance of Four Sectors

| | Energy (Quads) | Economic (Shipments $ Million) | Environment (Pollution Abatement $ Million) |
|---|---|---|---|
| Organics | 2.60 | $70,096 | 919 |
| Inorganics | 0.67 | $25,018 | 159 |
| Plastics & Synthetics | 0.89 | $55,635 | 465 |
| Agri-Chemicals | 0.67 | $20,899 | 99 |
| Percent of Chemical Industry Represented | 93% | 67% | 95% |

Source: *Manufacturing Consumption of Energy, 1994*. EIA, December 1997.

14

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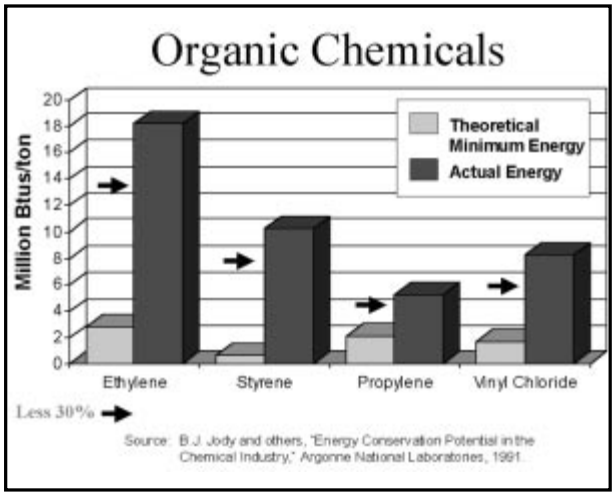
Organic Chemicals
Million Btus/ton
20
18
16
14
12
10
8
6
4
2
0
Theoretical Minimum Energy
Actual Energy
Ethylene
Styrene
Propylene
Vinyl Chloride
Less 30%
Source: B.J. Jody and others, "Energy Conservation Potential in the Chemical Industry," Argonne National Laboratories, 1991.

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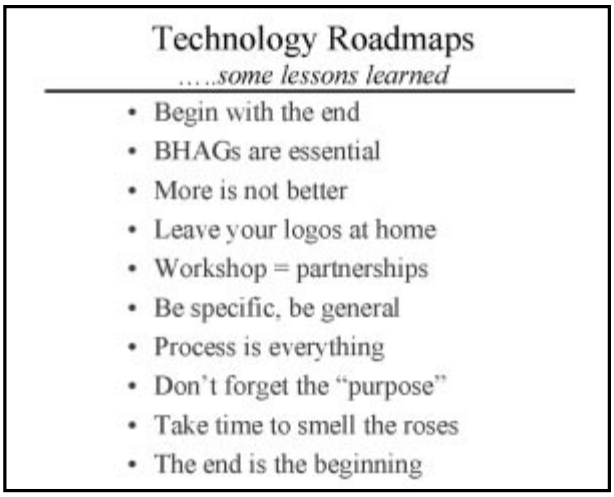
Technology Roadmaps
…..some lessons learned
• Begin with the end
• BHAGs are essential
• More is not better
• Leave your logos at home
• Workshop = partnerships
• Be specific, be general
• Process is everything
• Don't forget the "purpose"
• Take time to smell the roses
• The end is the beginning

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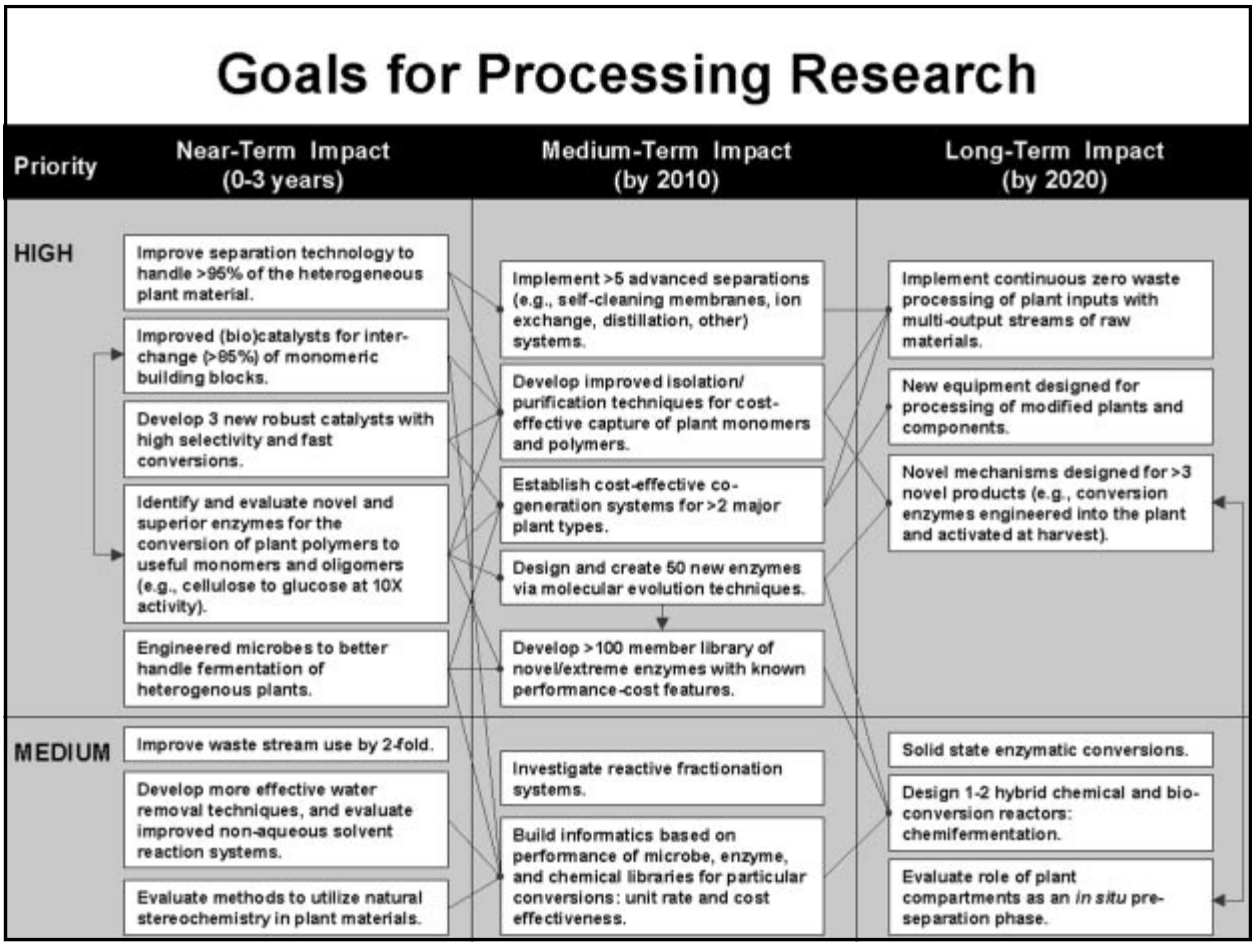
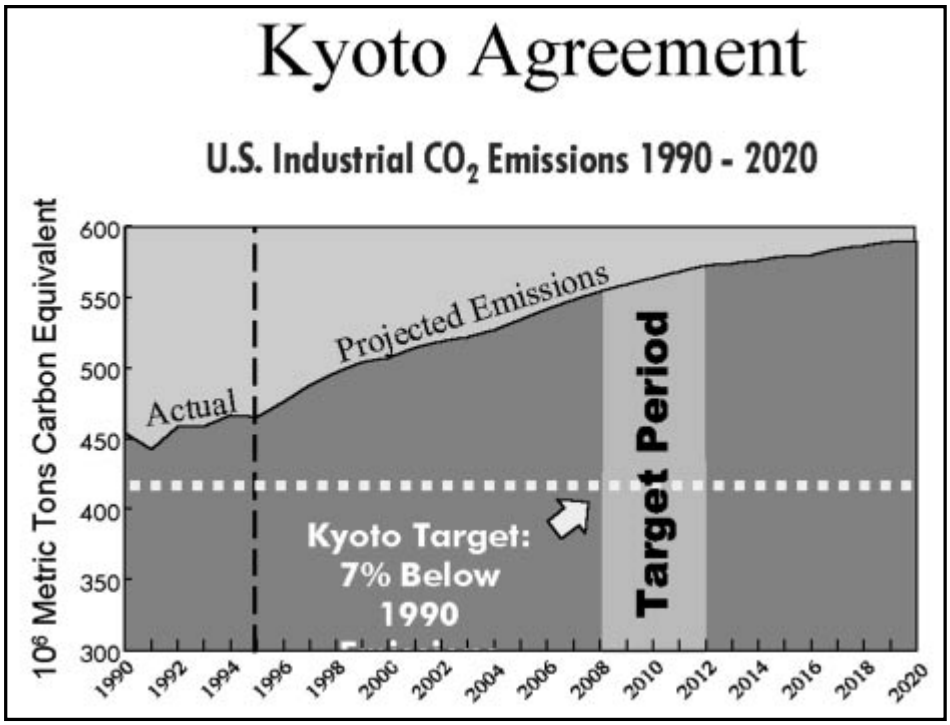

Goals for Processing Research
Priority
Near-Term Impact (0-3 years)
Medium-Term Impact (by 2010)
Long-Term Impact (by 2020)
HIGH
Improve separation technology to handle >95% of the heterogeneous plant material.
Improved (bio)catalysts for inter-change (>85%) of monomeric building blocks.
Develop 3 new robust catalysts with high selectivity and fast conversions.
Identify and evaluate novel and superior enzymes for the conversion of plant polymers to useful monomers and oligomers (e.g., cellulose to glucose at 10X activity).
Engineered microbes to better handle fermentation of heterogenous plants.
Implement >5 advanced separations (e.g., self-cleaning membranes, ion exchange, distillation, other) systems.
Develop improved isolation/ purification techniques for cost-effective capture of plant monomers and polymers.
Establish cost-effective co-generation systems for >2 major plant types.
Design and create 50 new enzymes via molecular evolution techniques.
Develop >100 member library of novel/extreme enzymes with known performance-cost features.
Implement continuous zero waste processing of plant inputs with multi-output streams of raw materials.
New equipment designed for processing of modified plants and components.
Novel mechanisms designed for >3 novel products (e.g., conversion enzymes engineered into the plant and activated at harvest).
MEDIUM
Improve waste stream use by 2-fold.
Develop more effective water removal techniques, and evaluate improved non-aqueous solvent reaction systems.
Evaluate methods to utilize natural stereochemistry in plant materials.
Investigate reactive fractionation systems.
Build informatics based on performance of microbe, enzyme, and chemical libraries for particular conversions: unit rate and cost effectiveness.
Solid state enzymatic conversions.
Design 1-2 hybrid chemical and bio-conversion reactors: chemifermentation.
Evaluate role of plant compartments as an in situ pre-separation phase.

18

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# Current and Future Issues in Reaction Engineering, by Lanny Schmidt

**"The chemical reactor is the heart of any chemical process."**

**The Engineering of Chemical Reactions**
**L. D. Schmidt**
**1998**

1

## Chemical Processes

1. The definition of chemists and chemical engineers is that they understand and manage chemical reactions.
2. Most interesting reactions involve catalysts, either man-made or biological.
3. Energy management is a dominant concern in most chemical processes.
4. Most chemical reactors involve multiple phases.
5. Mass and heat transfer usually limit the performance of industrial reactors.
6. Polymers and other fine chemicals and their intermediates represent the dominant current market for innovation and growth.
7. Materials and pharmaceuticals represent the dominant future market for innovation and growth.
8. The greatest potential for greenhouse gas reduction and pollution abatement comes from redesigning chemical reactors to produce less undesirable byproducts
9. The greatest safety hazard in chemical processing is the chemical reactor.

2

## Chemical Reaction Engineering in Trouble

1900–1950 Hougen and Watson
chemical processing units
integral balances

1955–1975 Amundson and Aris
analysis of chemical reactors

1975 Where to?
all easy problems analyzed
numerical simulations not generalizable

Breakthroughs

| | |
|---|---|
| polymer reactors | Harmon Ray |
| microelectronic reactors | Klavs Jensen |
| transport bed reactor | DuPont |
| metallocenes | Dow and Exxon |

3

## Chemical Processing "Units"

Dates from 1900 in England and the US

- reactor
- separators
- heat exchangers
- mixers
- pumps

The basis of flow sheet diagrams

4

## Outdated

Chemical reactors are almost omitted from process design texts

too complex to generalize

5

## The Key to New Technologies Is the Integration of "Units"

reactor + heat exchanger
- fluidized bed reactors
- multitube reactors
- phase change reactors

reactor + separator
- membrane reactors
- all multiphase processes

reactor + mixer
- microreactors
- emulsion

reactor + pressure drop
- pressure swing reactors

reactions under extreme conditions
- millisecond reactors
- microreactors
- high temperature
- high pressure
- supercritical

6

## Blurring Boundaries

- integration of units
- chemistry and engineering
- reaction engineering and catalysis
- reactor and heat and mass transfer
- experiment and theory
- modeling and simulation
- bench, pilot plant, and full scale
- steady state and transient
- commodities and fine chemicals

7

## Types of Processes

- petroleum
- commodity chemicals
- fine chemicals
- pharmaceuticals
- biochemicals
- materials
- foods

8

## Issues

- volume versus price
- need for new feedstocks
- need for new processes
- role of intellectual property
- growth and globalization
- environmental concerns

9

## Millisecond Chemical Reactors

Methane to syngas
  conversions and selectivities
  water addition
  staged reactors

Gasoline to syngas

Catalytic combustion

Catalytic wall reactor
  millisecond heat exchange
  radiant burner
  exothermic-endothermic reactors

Simulations

10

## Partial Oxidation

Exothermic
- autothermal

Large equilibrium constants
- fast
- complete reaction

Large gradients
- $10^5$ K/cm
- $10^7$ K/sec

Coupled processes
- surface reactions
- homogeneous reactions
- mass transfer
- heat transfer
- flow pattern

11

# Reaction Engineering 2020: An Academic Perspective, by Klavs Jensen

## Reaction Engineering - 2020
## An Academic Perspective

Klavs F. Jensen

Departments of Chemical Engineering and
Materials Science & Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

1

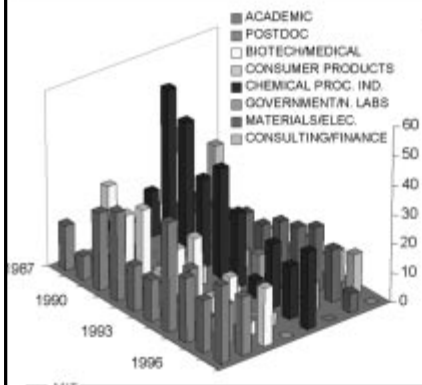
## Changes in the Chemical Industry

- The chemical industry is cyclical
- The industry is becoming increasingly global
- Mergers of companies and product lines
- Chemical companies are becoming life science companies and spinning o chemical units (Hoechst, Rhone Poulenc, DuPont…)
- Virtual companies - out-sourcing of services - incl. research
- Differentiation into
  - Knowledge based companies:
    - Product innovation in materials and life sciences
    - Solution partner - process outsourcing, supply management
  - Chemical utility (commodities)
  - Chemical service company
- *Reaction engineering needs to reposition itself to serve a diverse industry based on chemistry, biology, materials, electronics ...*

MIT

2

## PhD Employment 1987-1996




MIT graduates find jobs in a broad section of chemical, biological, and materials based companies.

MIT

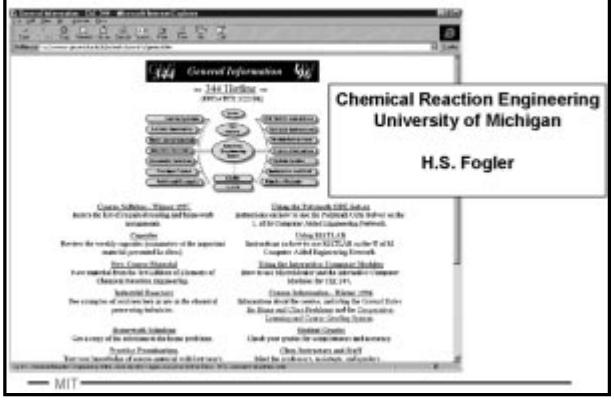
3

## Information Technology

- *Information technology will have an enormous impact on the way we teach and do research*
  - *Data bases*
  - *Data mining*
  - *Sharing of results and collaborative projects*
  - *Globalization*
  - *Education*
  -

4

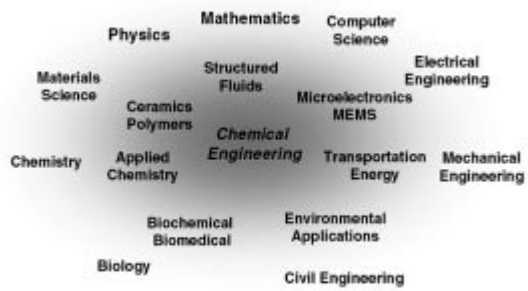
## Course Material and Teaching Using WWW




MIT

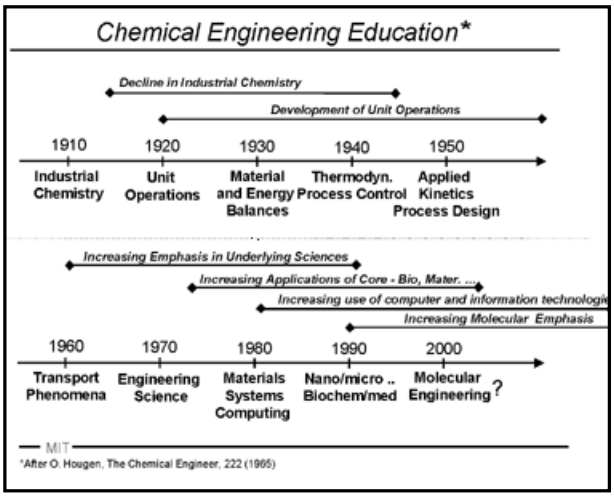
5

## Chemical engineering has a unique position at the interface between molecular sciences and engineering




Chemical reaction engineering integrates the key elements - kinetics, transport, thermodynamics in applications relevant to chemical, life science and materials applications

6


Chemical Engineering Education*
Decline in Industrial Chemistry
Development of Unit Operations
1910 1920 1930 1940 1950
Industrial Chemistry
Unit Operations
Material and Energy Balances
Thermodyn. Process Control
Applied Kinetics Process Design
Increasing Emphasis in Underlying Sciences
Increasing Applications of Core - Bio, Mater. ...
Increasing use of computer and information technologi
Increasing Molecular Emphasis
1960 1970 1980 1990 2000
Transport Phenomena
Engineering Science
Materials Systems Computing
Nano/micro .. Biochem/med
Molecular Engineering ?
MIT
*After O. Hougen, The Chemical Engineer, 222 (1965)

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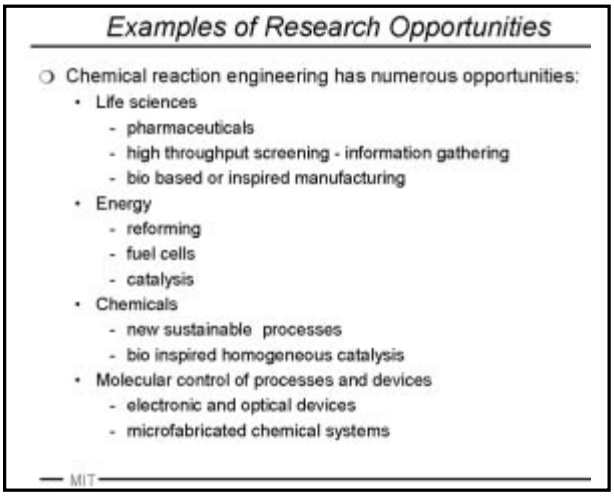
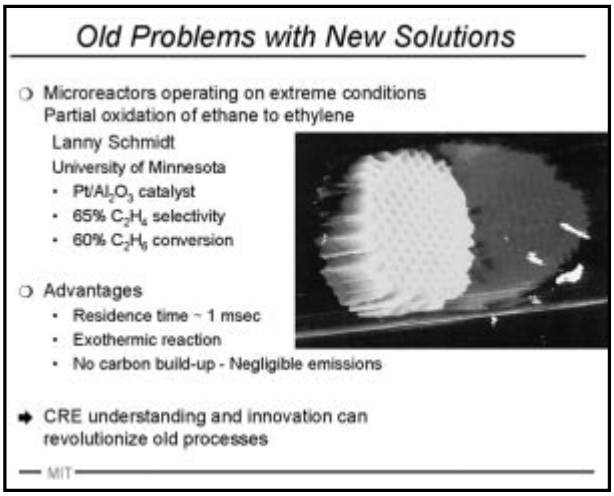
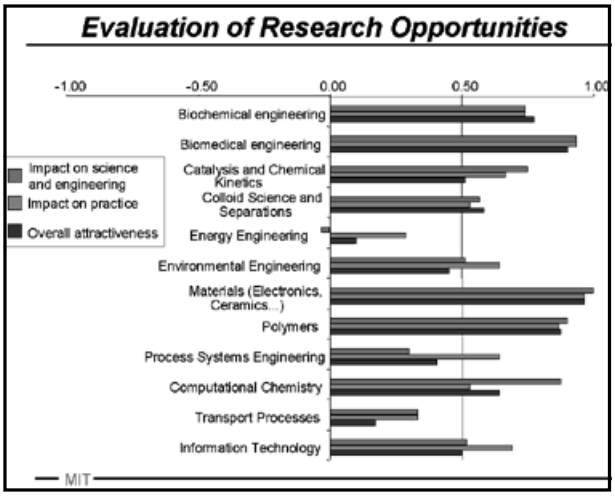

Examples of Research Opportunities
Chemical reaction engineering has numerous opportunities:
Life sciences
pharmaceuticals
high throughput screening - information gathering
bio based or inspired manufacturing
Energy
reforming
fuel cells
catalysis
Chemicals
new sustainable processes
bio inspired homogeneous catalysis
Molecular control of processes and devices
electronic and optical devices
microfabricated chemical systems
MIT

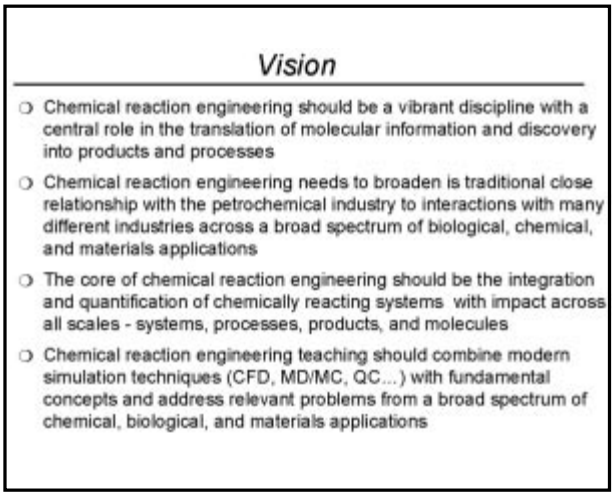
8


Old Problems with New Solutions
Microreactors operating on extreme conditions
Partial oxidation of ethane to ethylene
Lanny Schmidt
University of Minnesota
Pt/Al2O3 catalyst
65% C2H4 selectivity
60% C2H6 conversion
Advantages
Residence time ~ 1 msec
Exothermic reaction
No carbon build-up - Negligible emissions
CRE understanding and innovation can revolutionize old processes
MIT

9


Evaluation of Research Opportunities
-1.00 -0.50 0.00 0.50 1.00
Impact on science and engineering
Impact on practice
Overall attractiveness
Biochemical engineering
Biomedical engineering
Catalysis and Chemical Kinetics
Colloid Science and Separations
Energy Engineering
Environmental Engineering
Materials (Electronics, Ceramics...)
Polymers
Process Systems Engineering
Computational Chemistry
Transport Processes
Information Technology
MIT

10


Vision
Chemical reaction engineering should be a vibrant discipline with a central role in the translation of molecular information and discovery into products and processes
Chemical reaction engineering needs to broaden is traditional close relationship with the petrochemical industry to interactions with many different industries across a broad spectrum of biological, chemical, and materials applications
The core of chemical reaction engineering should be the integration and quantification of chemically reacting systems with impact across all scales - systems, processes, products, and molecules
Chemical reaction engineering teaching should combine modern simulation techniques (CFD, MD/MC, QC...) with fundamental concepts and address relevant problems from a broad spectrum of chemical, biological, and materials applications

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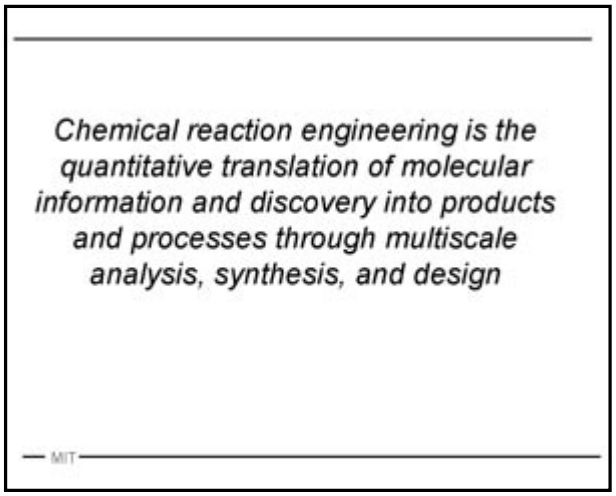
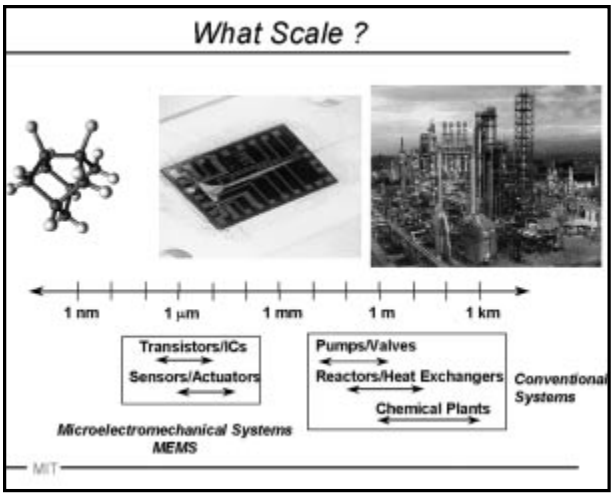

Chemical reaction engineering is the quantitative translation of molecular information and discovery into products and processes through multiscale analysis, synthesis, and design
MIT

12

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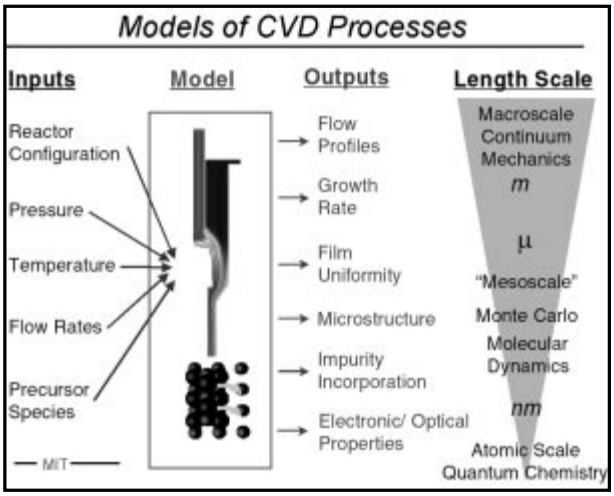


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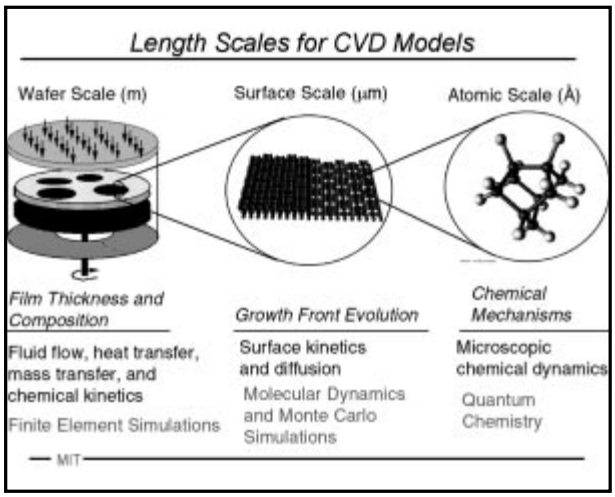


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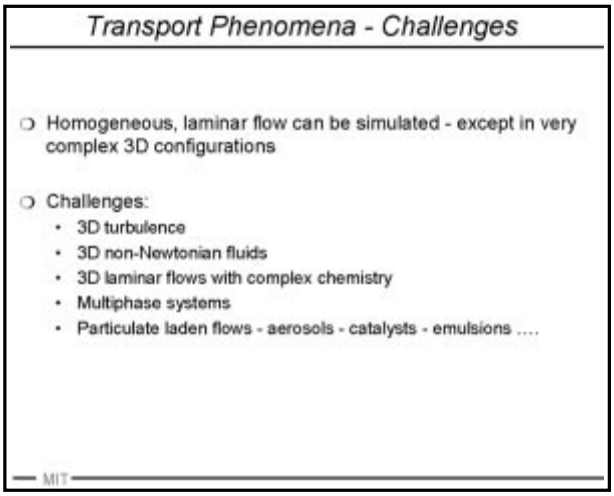


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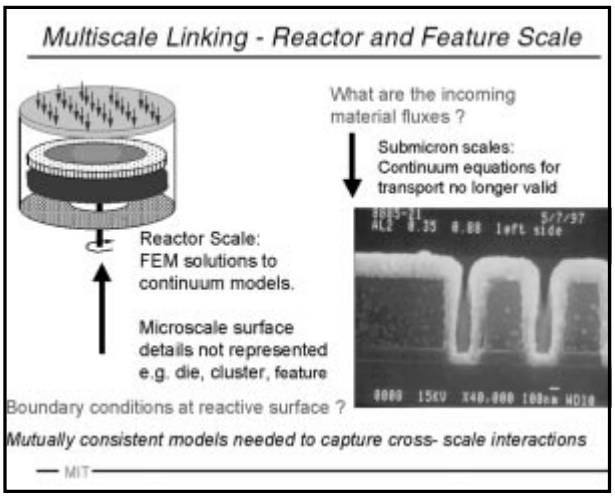


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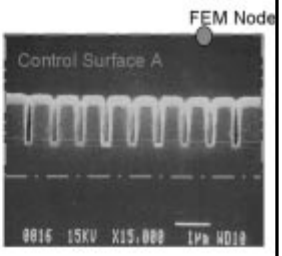
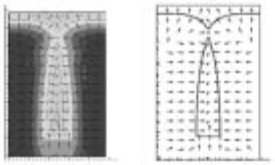
## Linking Method

- Link by flux balance - as in the classical Thiele modulus approach for heterogeneous catalysis, but with much more detail on the microscopic level



- Level set approach
- CRE should take advantage of the latest mathematical tools

MIT

19

## Quantum Chemistry Motivation and Methods

- Continued advances in processing require greater understanding and control of reactive processing at the molecular level
- Quantum Chemistry
  - Molecular structure and energetics
  - Thermodynamic properties: $\Delta H$, $\Delta S$, $\Delta G$,
  - Reaction parameters (with transition state theory): $K_{eq}, E_a, k_f$...
- Methods:
  - "*Ab Initio*": MP2, G2
  - "Density Functional Theory"
- Issues:
  - How accurate are the different methods?
  - Which methods are best for given problems?
  - How should we attack surface chemistry problems?
  - What size systems can be studied?
  - How do we link quantum mechanics to processing?

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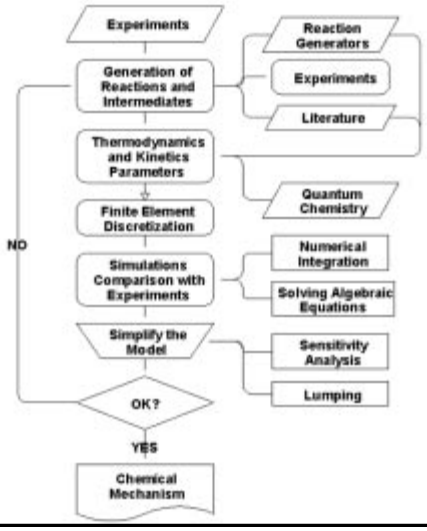
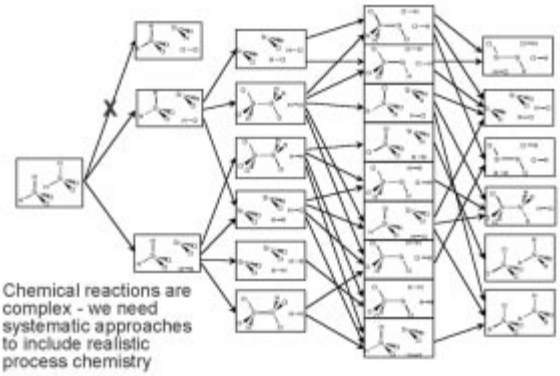
## Methodology for Chemical Mechanism Development




21

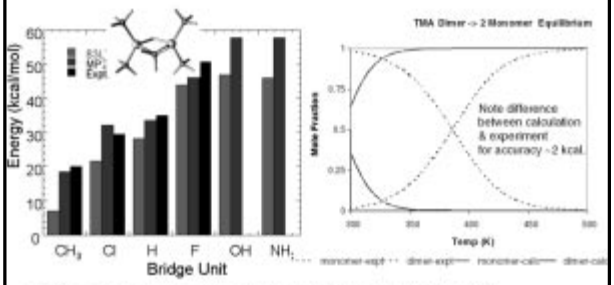
## Reaction Pathways in $SiH_2Cl_2$ (DCS) Decomposition



Chemical reactions are complex - we need systematic approaches to include realistic process chemistry

22

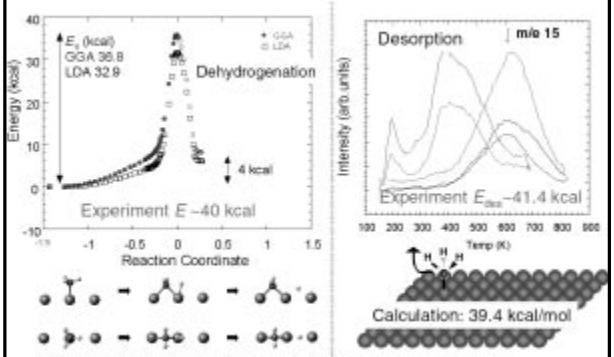
## Accuracy of Gas Phase QC Methods




- DFT methods consistently under-predict bridge bond strengths.
- Traditional *ab initio* methods perform well for these compounds.
- Consistent with the under-binding of bridge compounds, DFT methods underpredict unimolecular activation barriers

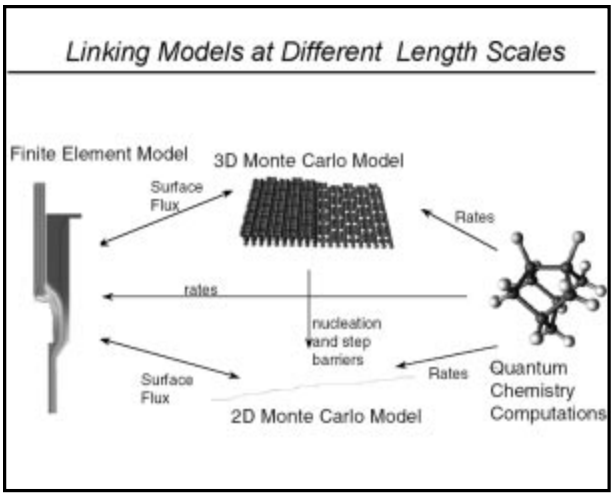
23

## Accuracy of Slab Calculations




- Comparison with experiments suggests an accuracy within ~ 5 kcal/mol - comparable to gas phase calculations.

24

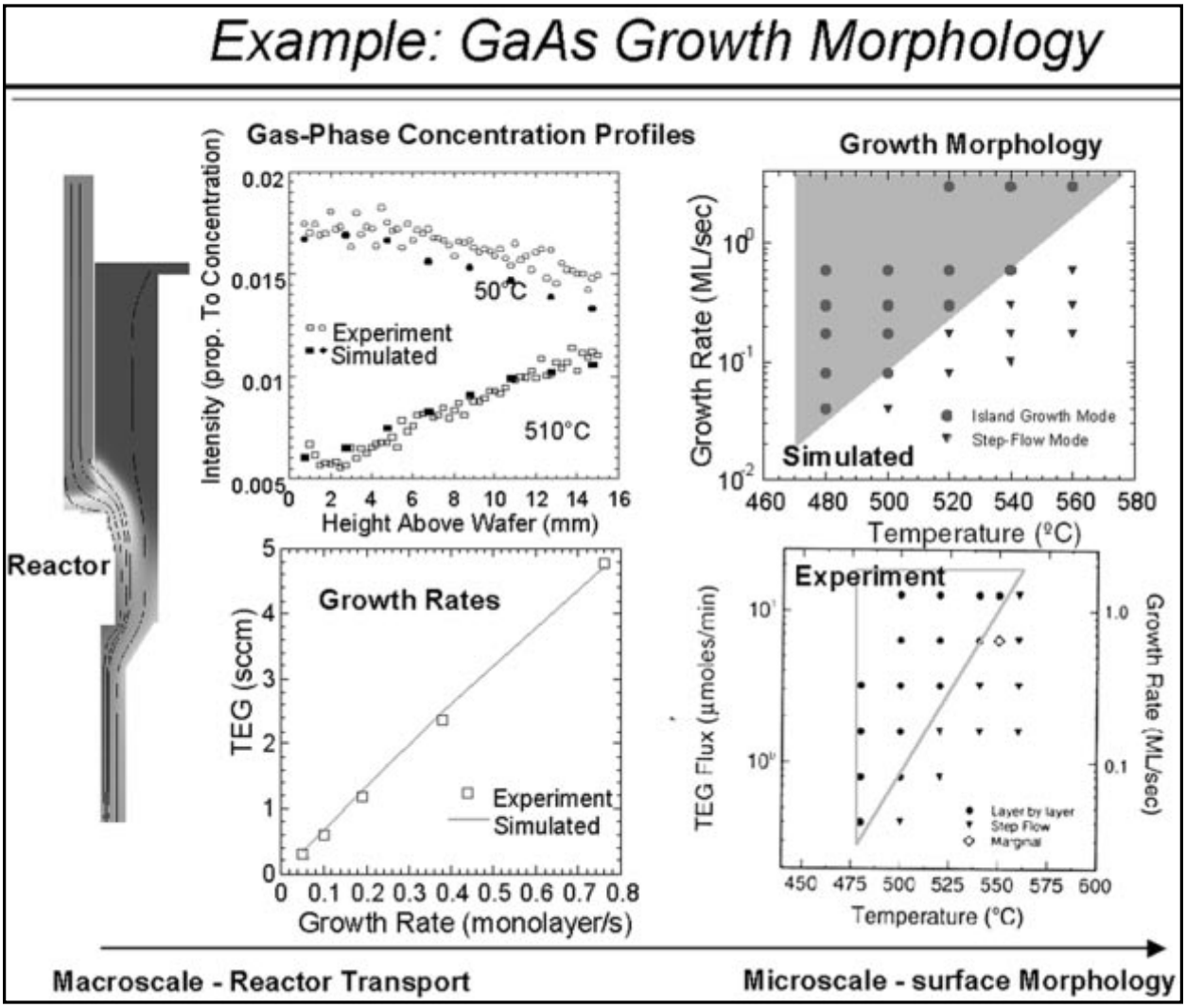



25

## Linking Across Scales - Challenges

- Methods for linking CRE models across length and time scales allow prediction of macro-and microscopic process performance measures - specifically macroscopic effects on morphology and ultimately performance
- Predictive models are becoming available for simulating macroscopic aspects of simple processes as well as limited structural features, but challenges remain:
  - Reaction generators - beyond hydrocarbons
  - Faster and calibrated QC methods
  - Robust method for handling 3D simulations with complex reaction mechanism
  - Surface processes - faster QC, MD, and MC approaches
  - Microscopic and atomic level data
  - Structure - property - performance relationships

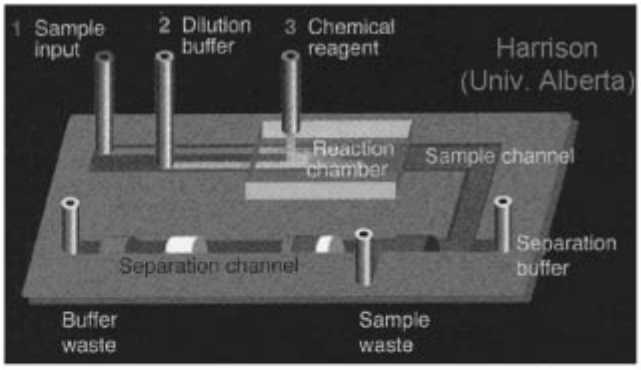
27

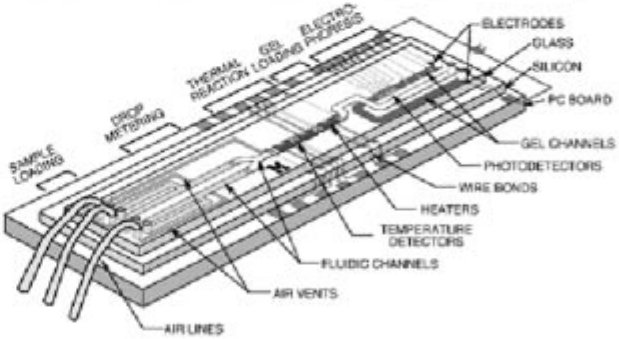


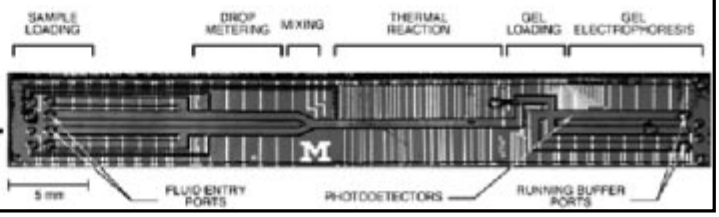

26

## μTotal Analysis Systems - "Laboratory On A Chip"

- Drug discovery
- Clinical diagnostics
- Advantages:
  - Small volumes
  - Parallel operation
  - Fast screening
- Examples:
  - Enzyme inhibition
  - DNA/RNA separation and sequencing
  - Receptor ligand binding
  - Immunoassay



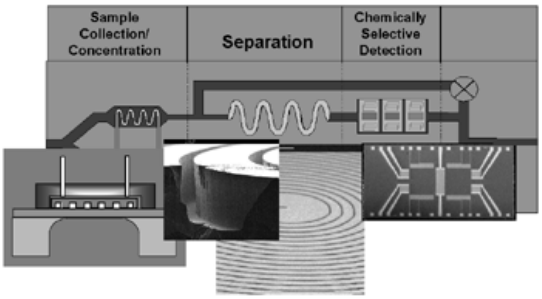

— MIT —

Burns *et al. Science*, **282**, 484 (1998)

28

## μChemLab™ Gas Phase Analysis System

**Sandia National Laboratories**




- The increased availability of miniaturized sensors will provide much needed data for CRE efforts

— MIT

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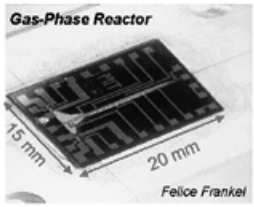
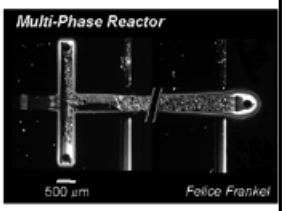
## MicroChemical Systems - Motivation




- Advantages:
  - Integration of chemical transformations with sensors and actuators
  - Portable, flexible, and smart devices
  - Packaged system for distributed - on demand - on time - manufacturing
  - Fast scale-up to production by replication
  - Safety - less inventory - safe handling of reactive, hazardous chemistry
  - Performance - access to extreme operating conditions
  - New methods for high throughput reaction/catalyst screening

30

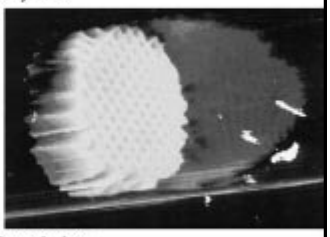
## Micro- and Meso-Chemical Reactors

- Microfabrication offers opportunities for realizing CRE designs with improved performance and high throughput
- Examples: fine chemicals [Merck (D)] and polymers [Aventi]

31

## Catalyst Monoliths as Microreactors

- Microreactors operating on extreme conditions
  Partial oxidation of ethane to ethylene
  Lanny Schmidt
  University of Minnesota
  - $Pt/Al_2O_3$ catalyst
  - 65% $C_2H_4$ selectivity
  - 60% $C_2H_6$ conversion



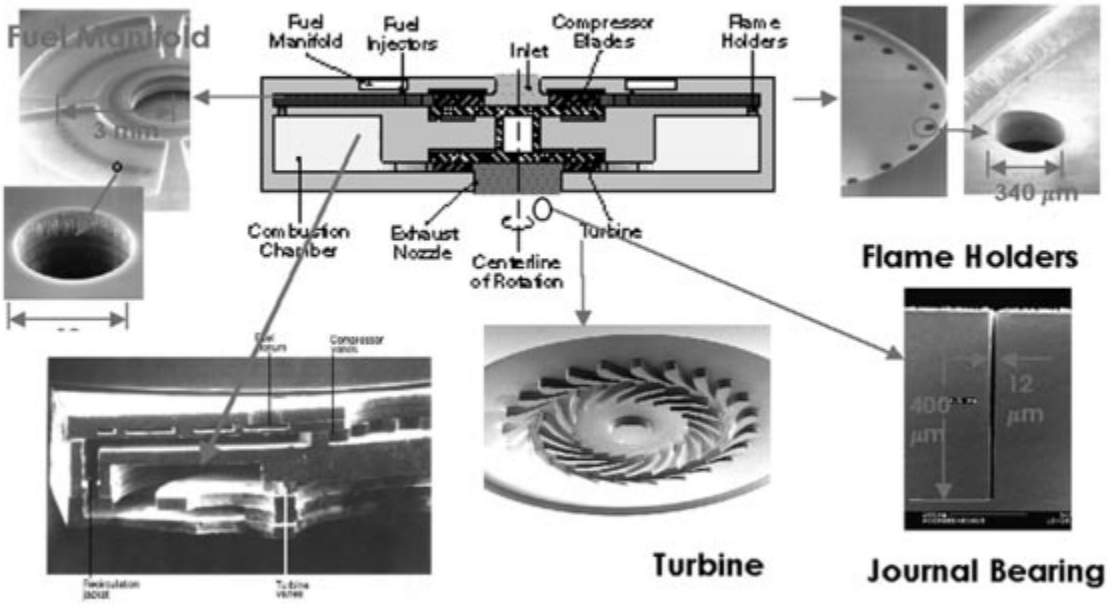
- Advantages
  - Residence time ~ 1 msec
  - Exothermic reaction
  - No carbon build-up - Negligible emissions

➡ CRE understanding leads to new reactors with much reduced volume

32

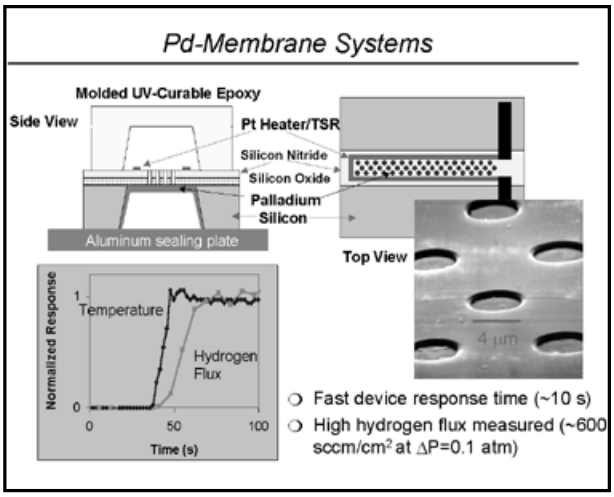
## MIT Microturbine Project

**- A. Epstein, I. Waitz, M. A. Schmidt *et al.***

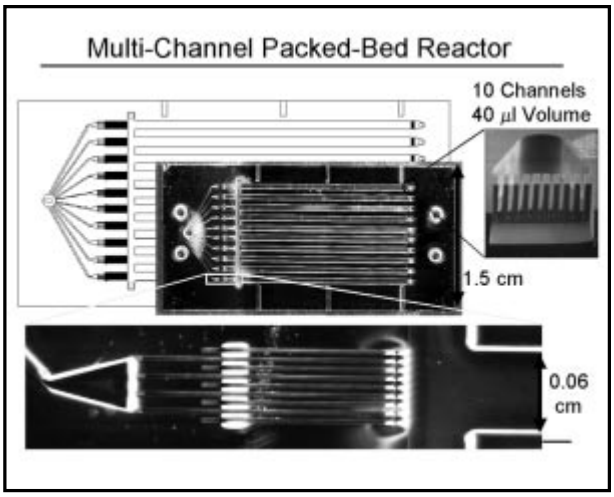



- Silicon micromachining allows prototyping of complex integrated systems

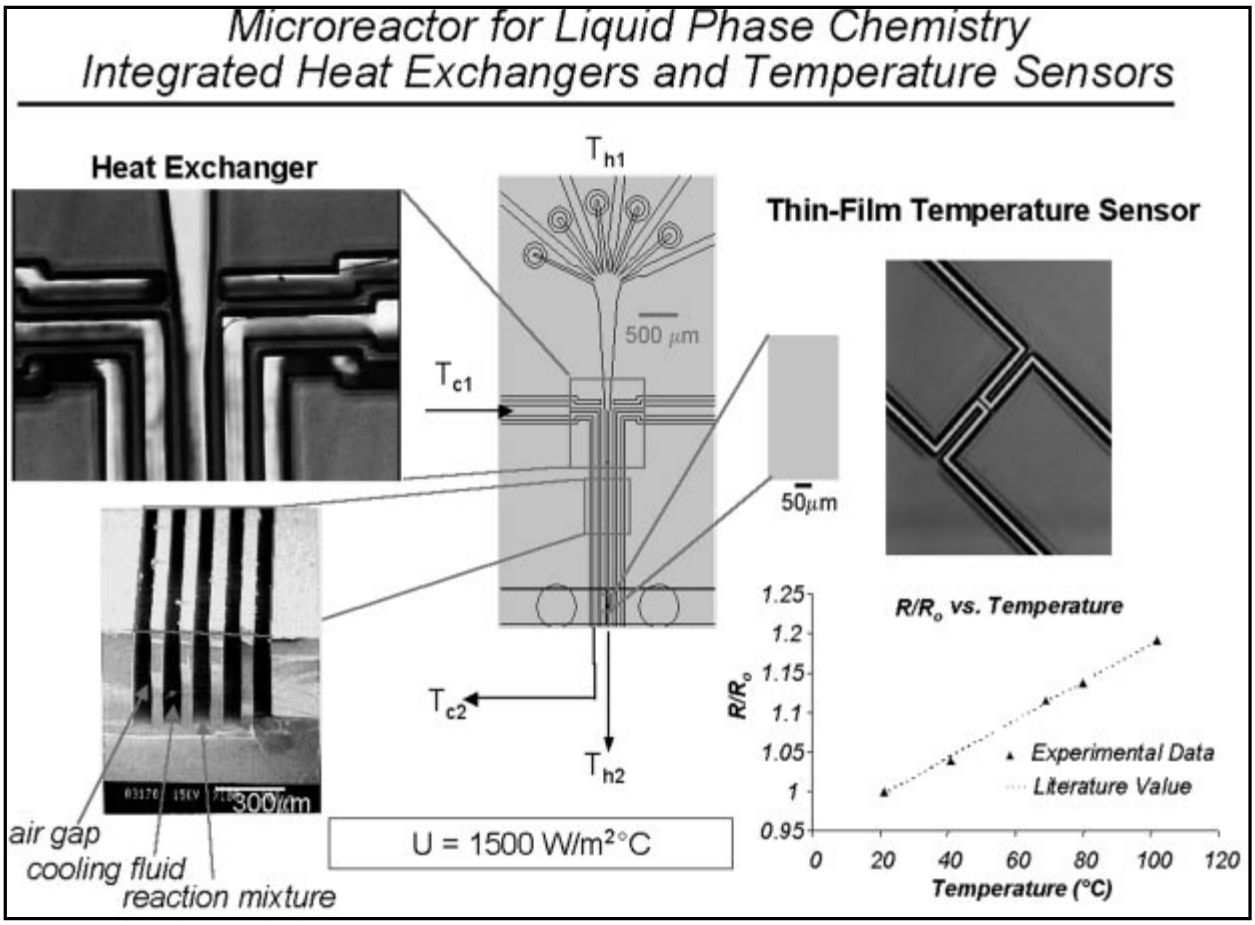
33


Pd-Membrane Systems
Molded UV-Curable Epoxy
Side View
Pt Heater/TSR
Silicon Nitride
Silicon Oxide
Palladium
Silicon
Aluminum sealing plate
Top View
4 μm
Normalized Response
Temperature
Hydrogen Flux
Time (s)
Fast device response time (~10 s)
High hydrogen flux measured (~600 sccm/cm² at ΔP=0.1 atm)

34

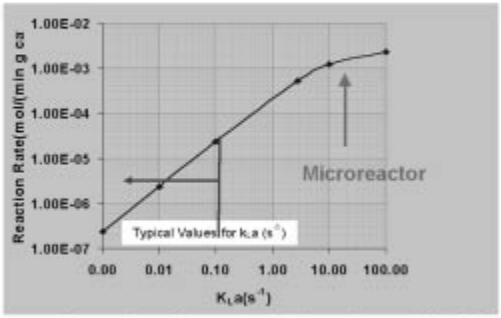

Multi-Channel Packed-Bed Reactor
10 Channels
40 μl Volume
1.5 cm
0.06 cm

36


Microreactor for Liquid Phase Chemistry
Integrated Heat Exchangers and Temperature Sensors
Heat Exchanger
Thin-Film Temperature Sensor
500 μm
50μm
300μm
air gap
cooling fluid
reaction mixture
U = 1500 W/m²°C
R/R₀ vs. Temperature
Experimental Data
Literature Value
Temperature (°C)

35

## Multiphase Microreactor Mass Transfer Characteristics




- Improved mass transfer means that reactor could be 100 fold smaller for the same production rate
- Opportunities for CRE to design novel reactors and processes

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## Summary

- Chemical reaction engineering (CRE) has many opportunities
  - the tools to incorporate realistic chemistry into models are becoming sufficiently powerful
  - computational fluid dynamics tols are maturing
  - microfabrication techniques can realize controlled contacting patterns in materials used for chemical reactors
  - new applications in materials and life science
- CRE needs to expand beyond its traditional focus and include synthesis and design

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# Reaction Engineering 2020: An Industrial Perspective, by Jan J. Lerou

## Economic Environment

- Imperative for all companies: GROWTH
  - Reality: CPI grows slowly
  - CPI Reaction: grow via Mergers & Acquisitions
- New rules for the global chemicals industry:
  - Globalization
  - Specialization
  - Consolidation
- In the US: Wall Street is OK with growth through M&A but we'll watch!

  Meaning: improve your results via rationalizations

1

## Economic Environment

Merger & Acquisition Activities:

- Oil:
  - BP/Amoco/Arco
  - Exxon/Mobil
- Commodities:
  - Paper: International Paper/Unisource
  - Aluminum: ALCAN/Pechiney/Alusuisse
  - Chemicals: Dow/Union Carbide
- Pharmaceuticals:
  - Hoechst/Rhone-Poulenc-Rorer
  - Zeneca/Astra

2

## Economic Environment

Another trend:

From chemicals to life sciences!

- Monsanto
- Rhone-Poulenc
- Hoechst
- DuPont

WHY?

- To arrive at less cyclical businesses
- To become a "sustainable growth" company
- To become more environmentally friendly

3

## Economic Environment

What are the consequences for Chemical Engineering and for Reaction Engineering?

- Continuous reorganizations and mergers initially cost jobs.
- Uncertain future causes engineering students to turn away from chemical engineering.
- Within companies future of process engineers looks dim.
- Classical chemistry and chemical engineering lost appeal.

Is there only gloom and doom?

or

Is there light at the end of the tunnel?

4

## Scenario for the future

A bright future:

Because how can one

- arrive at less cyclical businesses
- become a "sustainable growth" company
- become more environmentally friendly

without a fundamental understanding of the manufacturing processes, be that chemical, biochemical, biological etc.?

5

## Case Study: DuPont

From "Better Things for Better Living" to

"The Miracles of Science™"

Why this new slogan?

Because DuPont wants to emphasize the importance of science to our past while capturing the promise of new and exiting things yet to come.

We have always been a science company because we bring science to the market in ways that help make people's life better.

Now, we take it a step further and are building competencies beyond physics and chemistry to include biotechnology and information technology.

6

## Case Study: DuPont

Why this change of direction?

- DuPont used to focus on inventing and perfecting polymers and other materials that mimic natural materials and/or offer enhanced or new properties that are not possible with natural materials: Nylon, Lycra, Corian, Kevlar, Teflon etc.
- Our processes consumed large amounts of depletable forms of natural resources and energy and co-produced unwanted products.
- We are now transforming the way in which we create value for society and our shareholders by creating more value with less impact.
- The belief is the biotechnology will facilitate and accelerate this transformation.

7

## Case Study DuPont

DuPont walks the talk....

DuPont and MIT have signed a memorandum of understanding to form a $35 million, five-year alliance to advance research and education in materials from biotechnology that have a variety of applications. The five-year alliance will begin Jan. 1, 2000.

This alliance will support projects that draw upon the science, engineering, and business expertise at MIT and that extend and better leverage the reach of DuPont's scientific expertise in the areas of biology, genetics, bioinformatics and catalysis. It will bring together DuPont's and MIT's strengths in materials, chemical and biological sciences to develop new processes for new materials directed at bioelectronics, biosensors, biomimetic materials, alternative energy sources and new high-value materials.

9

## Consequences for CRE

- More Bioreaction Engineering
  - Biotechnology is clearly on the upswing
  - Bioprocessing
  - Bioreactors & bioseparations
  - Bioprocess modeling
  - Biocatalysis
- Alternative processes
  - Less capital intensive
  - Use renewable raw materials
  - Zero waste
  - Novel reactors
  - Intensification & Miniaturization

10

## Consequences for CRE

- Emphasis on Asset Productivity
  - More fundamental understanding
  - Improved catalysis for selectivity
  - More process modeling
  - More 6 Sigma approaches
  - Novel sensors
  - Improved process control

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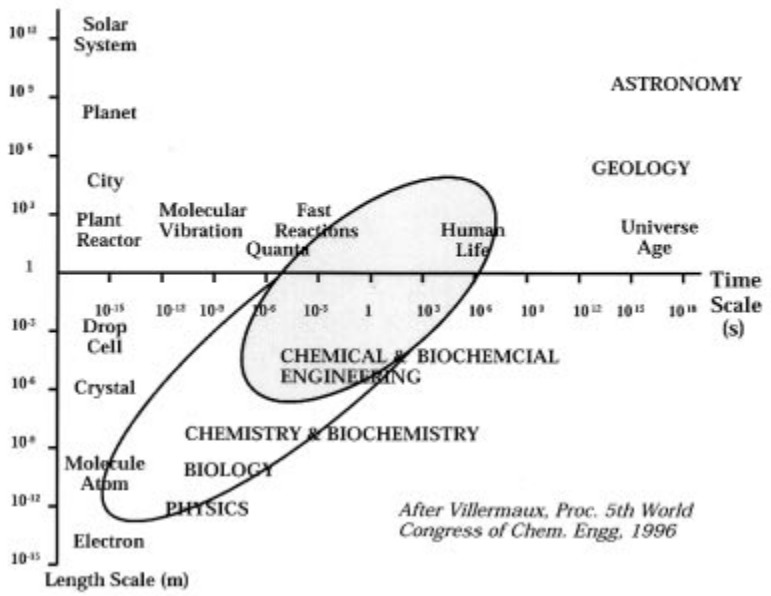
## Space and Time Scales




12

## The 21st Century….

- Ample opportunities for chemical reaction engineers.
- Keywords are creativity & flexibility to address a rapidly changing economical environment.
- Between now and 2020 will be an extremely interesting and challenging time for our profession and ourselves…

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# Reaction Engineering in a Process Context, by Herman DeMeyer

## Chemical Process Context

General

- Analysis of processes for
  established market products - specifications
- Incremental improvements - small margins
- Redesign
- Design cycle very short, little engineering impact
  Pharmaceutics, Phyto-pharmaceutics, Bio, …
- Economics of model-based activities

1

## Chemical Process Context

Targets and Tools

- "Complete" kinetics
  Side reactions in ppm range, color-precursors, …
  Reconciliation of lab- and plant-data
- Dynamic models
  Operation procedures and exceptional process-states
  Optimal design, constrained by "standards", …
  Control as well as layout, mass- and energy-balances
- Dynamic on-line optimization

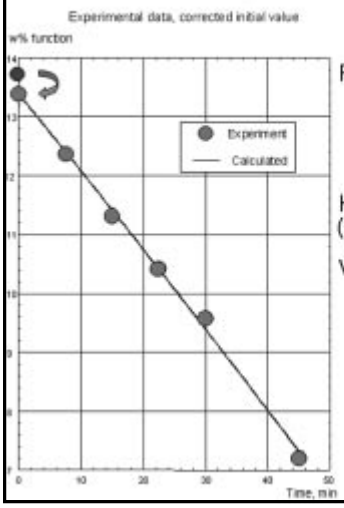
2

## Kinetics

- Chemical reaction at heart of the design
  - formal kinetic relationships based on mechanism
    → basis for plausibility/validation of side-reactions, …
  - hypothesis & mechanism generator
    → integrated & interactive database of alternatives
    → discriminating optimizer for culling and experiment planning
    → "combinatorial" kinetics
  - extension of consistency check with plant-data
    → homogeneous combination of data from lab & plant
    → "Data-mining" from industrial, prototype or miniplant(s) to complement and cross-check

3

## Kinetics example




Reaction

$A + B \rightarrow C + D$

Homogeneously catalized (Kat)

Very complicated analytics

4

## Kinetics example

- In this case the formal rates of C-production prove useful:

| | |
|---|---|
| $r_C = k_0$ | no mechanistic background |
| $r_C = k_1 \cdot C_A / (1 + K_1 \cdot C_A + K_C \cdot C_C)$ | building complex A-Kat |
| $r_C = k_2 \cdot (C_A \cdot C_B - C_C/K) / (1 + K_1 \cdot (C_A + C_B) + K_C \cdot C_C)^2$ | attack of B by A-Kat |
| $r_C = k_{2M} \cdot (C_A \cdot C_B - C_C/K) / (1 + K_1 \cdot C_A \cdot C_B)$ | release of C-Kat |

- Selection out of ~100 possibilities
- Fit is equally good for lab-results,
- The use of the expressions for the industrial reactor:
  Variance of more than 1000% in residence-time

5

## Kinetics

A system approach to reaction analysis

- uncertainty not as an analysis, but as a design tool
- inclusion of physical & thermodynamic effects
  → flow-determining factors, gas- and solid-formation
  → formal analysis of batch/continuous differences
- catalysis homogeneous/inhomogeneous
- solvent effects
- early determination of design-determining step
  → factoring, quantification & ranking of phenomena

6

## Kinetics example

Solvent S

| | |
|---|---|
| $A_n + B \rightarrow C + D$ | quick & endothermic |
| $D\,(S) \leftrightarrow D\uparrow\,(Gas)$ | phase-transfer resistance |
| $B\,(S) \leftrightarrow B\uparrow\,(Gas)$ | highly nonideal |
| $S_{liq} \leftrightarrow S\uparrow\,(Gas)$ | |
| $C\,(S) \leftrightarrow C\downarrow\,(Solid)$ | |
| $A_n + D \leftrightarrow E_n$ | very quick, exothermic |
| $E_n + i\,D \leftrightarrow F_n\,(Gel) + H$ | thixotropic |
| $E_n\,(S) \leftrightarrow E_n\downarrow\,(Solid)$ | |
| $A_n + C \rightarrow L\downarrow\,(Solid)$ | heat-transfer |
| $A_n + j\,B \rightarrow J + j\,D$ | very quick, highly exothermic |
| $A_n + J \rightarrow H\downarrow(Solid)$ | $\Delta T$ |
| $C \leftrightarrow P + 2\,D$ | exotherm |
| $A_n + P \rightarrow N_a\downarrow\,(Solid)$ | quality |
| $\rightarrow N_b$ | |
| $\rightarrow N_c\,(Gel)$ | |

7

## Kinetics example

- Which phenomenon will determine the design
  - the quick initial parallel/competitive reaction-set
  - the gas-bubbles, gel/solid formation and non-Newtonian flow
  - the consecutive reactions and back-mixing
  - the nonideal gas-phase and phase-transfer resistance
  - the mixing and the locally inhomogeneous liquid
  - the heat-transfer and secondary deposit-building reactions
- Which reactor-type will be kept in mind
  - a stirred tank allowing degassing, but maximum feedback
  - will a strirrer be effective given the gel, gas and solid
  - a tubular reactor allowing parallel reactions

8

## Kinetics example

- One methodology may consist in consideration of all
  - treat as extra uncertainties with a specific distribution
  - use validation and expected physical distribution to eliminate
  - design experiments to eliminate distributions, not parameters
- All the information is available from the "kinetics"

9

## Reactor modeling

Economics of the modeling effort

- Systematic treatment of
  - 4-phase systems
  - Ionic, non-aqueous and mixed systems
- Formal analysis to identify flowsheet problems
- Build-in handling of discrete events
- Natural interfacing/integration of CFD
  - non-Newtonian flow
  - turbulence
  - cooperative computing

10

## Reactor modeling

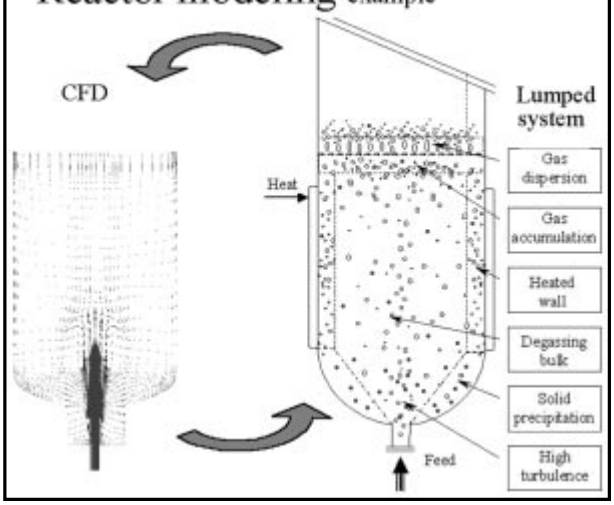
Economics of the modeling effort

- Consistent derivation of

  metrics, models, constraints and targets for
  - design
  - on-line (dynamic) optimization and
  - control
- Design specification as a "driver" for the design

11

## Reactor modeling example




12

## Reactor modeling example

- Split-physics
  - lumped model with physical proporties doing
    - chemistry
    - thermodynamics
    - phase transfer - heat transfer
    - Systems of ~100 chemicals, 3 phases in 5-100 "virtual" zones
  - finely gridded CFD generating
    - velocity fields
    - lumped flows at all "virtual" zone boundaries
    - metrics to judge placement, size of "virtual" zones
- Cooperative computing

13

## Conclusion

- As the Quechua-Inca put it
  only one thing is to be kept in mind:
  ama quella do not be lazy
- Ideas are available
- Technology is available
- Market is available
- Let us use time well!

14

# Knowledge Management: Needs and Opportunities, by Gregory J. McRae

## Knowledge Management

- Needs and Opportunities

Gregory J. McRae

MIT Chemical Engineering

1

## A Comparison – The Computer Industry

- 2 x Computer power every 18 months
- 2 x Parallel computing advances every 9 months
- 2 x Communications bandwidth every 18 months

➡ > 1000 fold increase in 20 years!!

3

## Vision 2020 Goals

**30% Reductions in:**

- Energy usage
- Raw materials
- Water consumption
- Toxic emissions
- Pollution

➡ 30% improvements in 20 years or 1.3% / year – are very low goals!

2

## Waste Generation by Industry Segment

| Industry Segment | Product Tonnage | Waste generation (kg byproducts/ kg product) |
|---|---|---|
| Oil Refining | $10^6$-$10^8$ | ~ 0.1 |
| Bulk Chemicals | $10^4$-$10^6$ | 1 - 5 |
| Fine Chemicals | $10^2$-$10^4$ | 5 - 50 |
| Pharmaceuticals | $10^1$-$10^3$ | 25 - 100+ |

4

## Vision 2020 Goals – Additional Factors

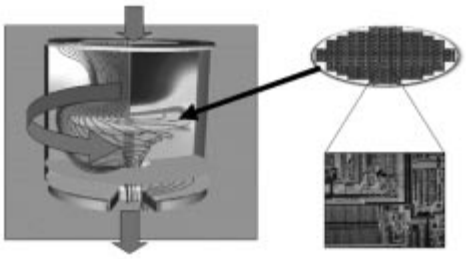
There are important issues beyond just the technology

- A broader view of reaction engineering
- Reducing the time to market is crucial
- Knowledge and information management
- Decision making and resource allocation in the presence of uncertainties
- Educational implications

5

## Example – Manufacture of Microelectronics

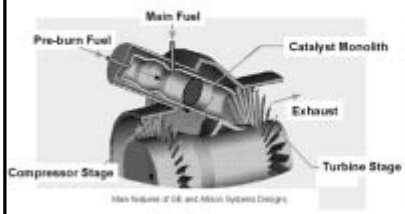
The Challenge: How to improve the process and reduce time to market?



6

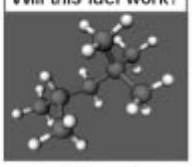
## Example - Catalytic Combustion (Multi-Scale)

The Challenge: Improve efficiency and reduce pollutant emissions ($NO_x$)




O(m)

Will this fuel work?

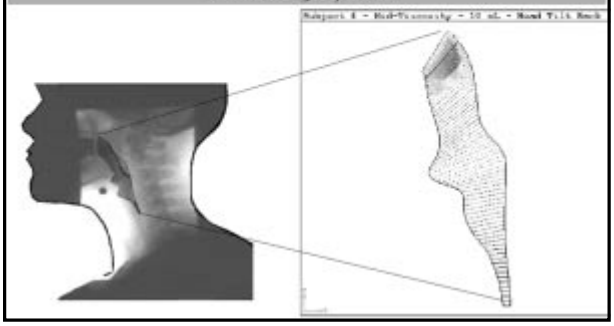


O(nm)

7

## Example – Biomedical Processes

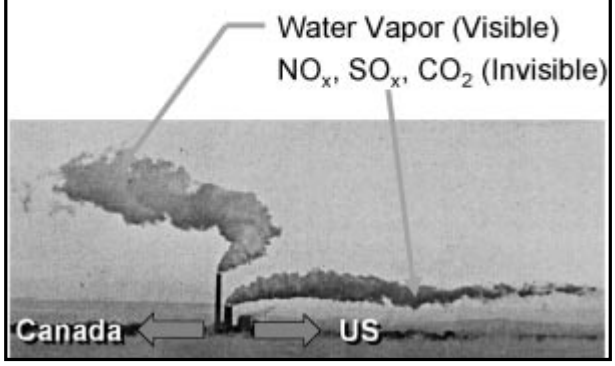
The Challenge: Understand complex fluid flows and drug uptake



8

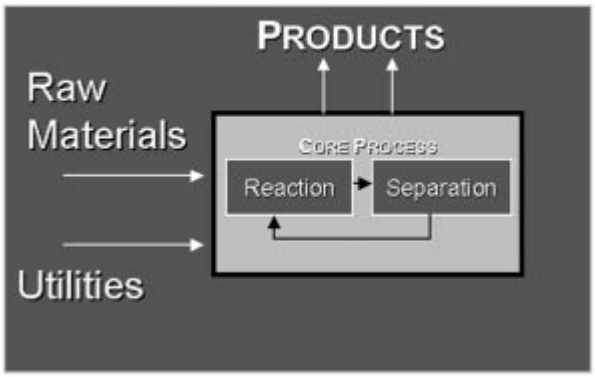
## Example -- Policy Implications

The Challenge: Develop cost-effective policies




9

## Process Engineering Viewpoints (1960's)

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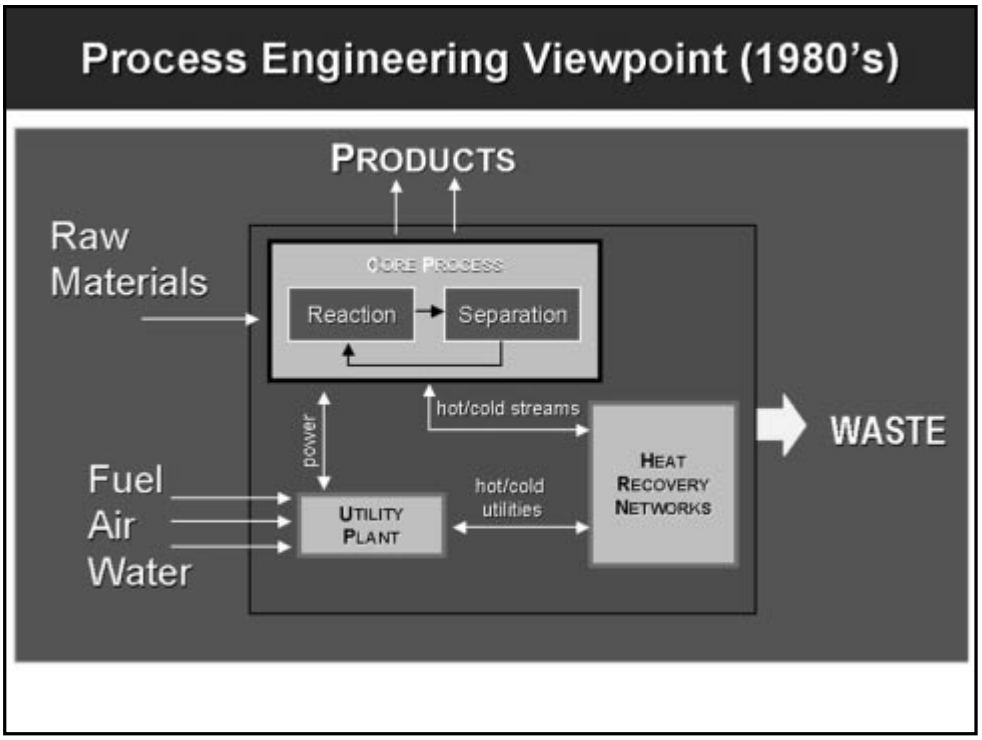
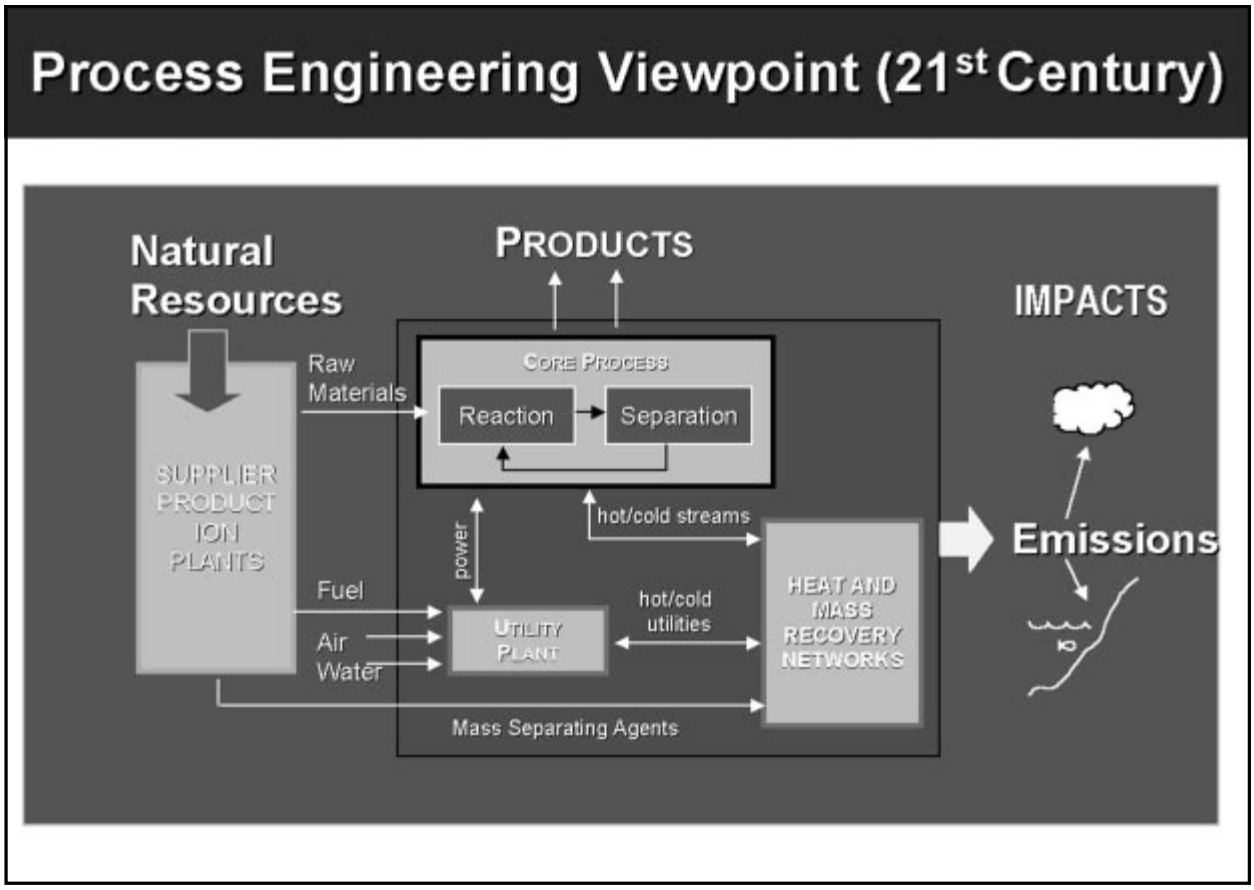

Process Engineering Viewpoint (1980's)
PRODUCTS
Raw Materials
CORE PROCESS
Reaction
Separation
hot/cold streams
power
WASTE
HEAT RECOVERY NETWORKS
Fuel
Air
Water
UTILITY PLANT
hot/cold utilities

11


Process Engineering Viewpoint (21st Century)
Natural Resources
PRODUCTS
IMPACTS
Raw Materials
CORE PROCESS
Reaction
Separation
SUPPLIER PRODUCTION PLANTS
hot/cold streams
power
Emissions
Fuel
Air
Water
UTILITY PLANT
hot/cold utilities
HEAT AND MASS RECOVERY NETWORKS
Mass Separating Agents

12

RETHINKING THE PROBLEM STATEMENT:

1. NEW PRODUCT DEVELOPMENT WITH THE ENVIRONMENT AS AN OBJECTIVE NOT AS A CONSTRAINT ON OPERATIONS

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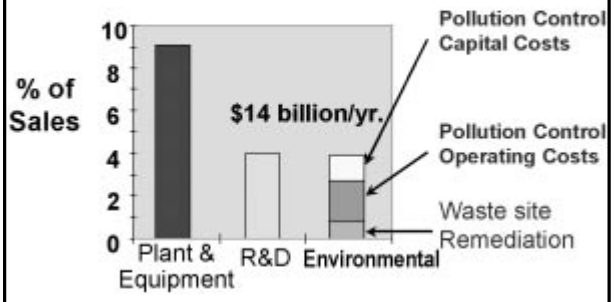
## U.S. Capital and R&D Expenditures



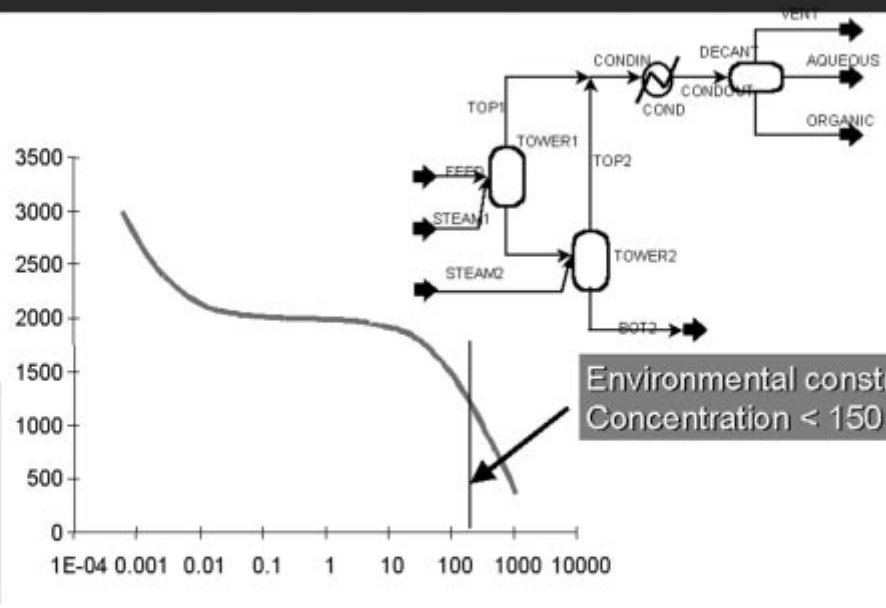

*Source of data: 1997 Chemical Manufacturers Association Economic Survey

14

## Tradeoffs Between Operation /Environment

Steam feed rate (lb/hr)

Impact of combustion products from boiler

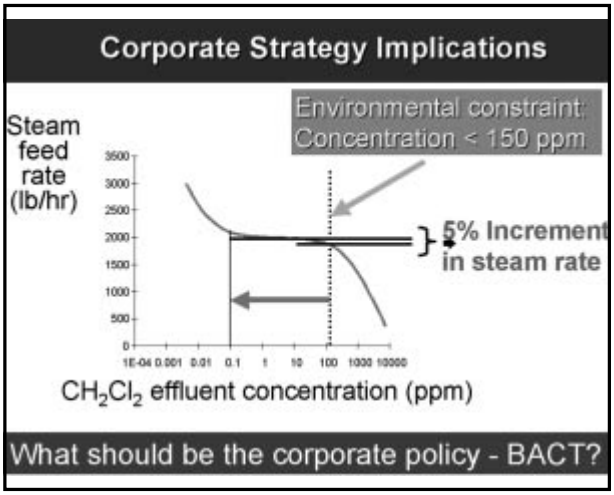



Environmental constraint: Concentration < 150 ppm

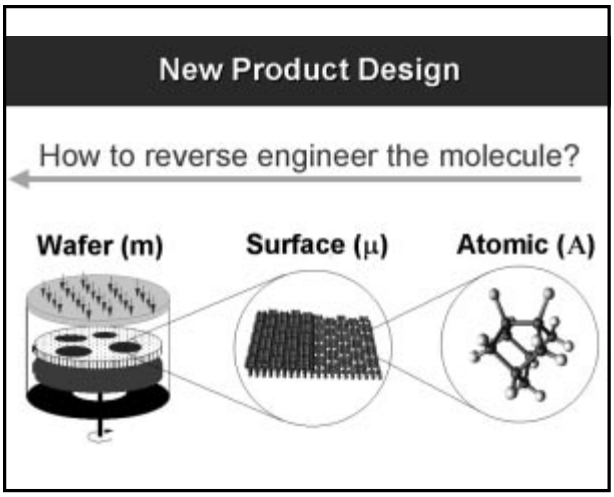
$CH_2Cl_2$ effluent concentration (ppm)

Impact of solvent releases

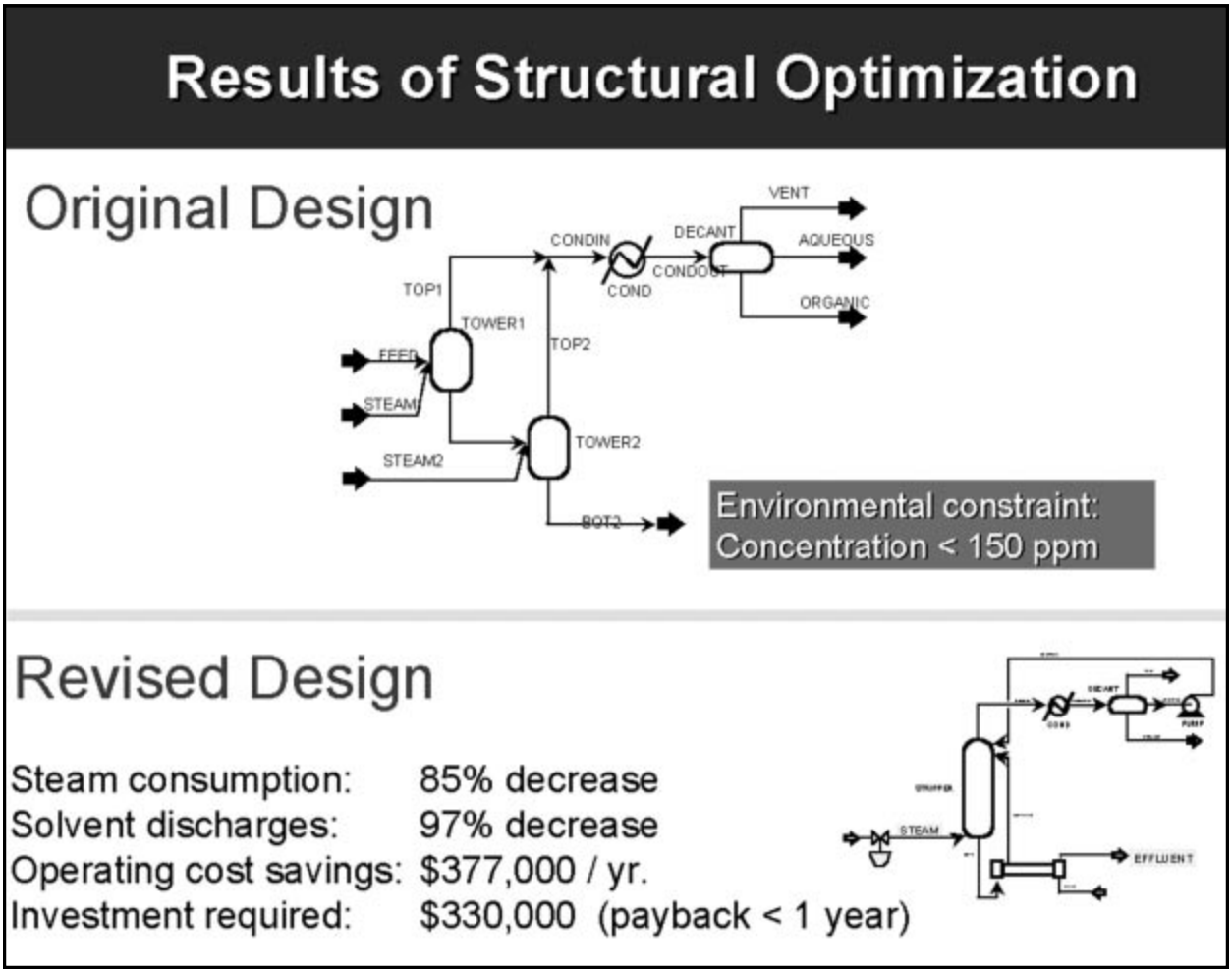
15


Corporate Strategy Implications
Environmental constraint:
Concentration < 150 ppm
Steam feed rate (lb/hr)
5% Increment in steam rate
$CH_2Cl_2$ effluent concentration (ppm)
What should be the corporate policy - BACT?

16


New Product Design
How to reverse engineer the molecule?
Wafer (m)
Surface (μ)
Atomic (A)

18


Results of Structural Optimization
Original Design
VENT
CONDIN
DECANT
AQUEOUS
CONDOUT
COND
TOP1
ORGANIC
TOWER1
TOP2
FEED
STEAM1
TOWER2
STEAM2
BOT2
Environmental constraint:
Concentration < 150 ppm
Revised Design
Steam consumption: 85% decrease
Solvent discharges: 97% decrease
Operating cost savings: $377,000 / yr.
Investment required: $330,000 (payback < 1 year)
STEAM
EFFLUENT

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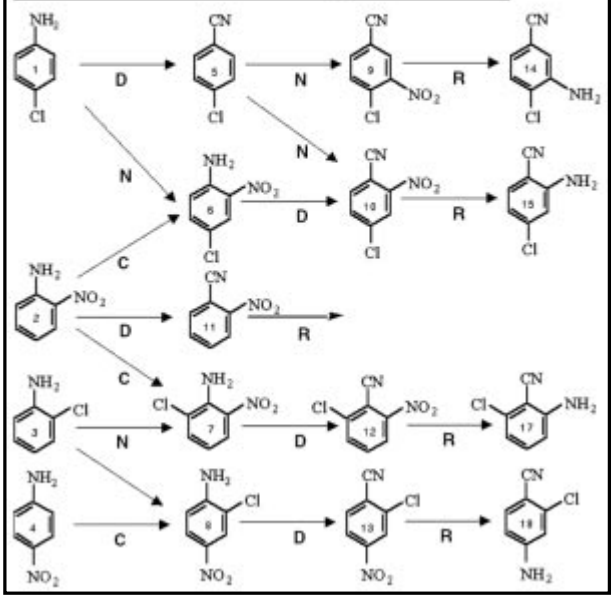
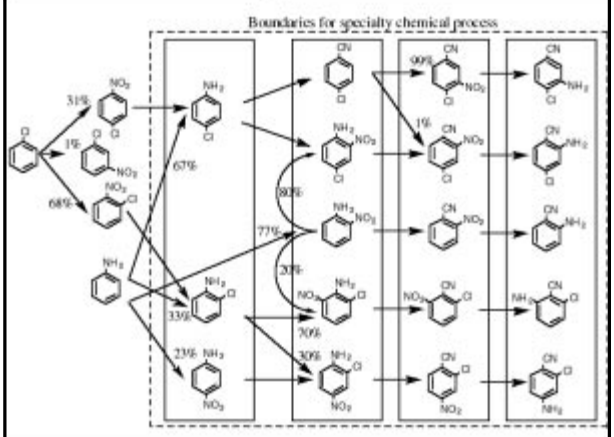
## Strategic Decisions - Reaction Path Synthesis



19

## Multiple Products - Business Integration




**Integrated production**
(Wastes cut by 1/3, Profit doubled)

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KEY ROLE OF INFORMATION TECHNOLOGY AND MANAGEMENT:

2. SEAMLESSLY INTEGRATING THE PROBLEM STATEMENT, MULTIPLE SOFTWARE SYSTEMS, PEOPLE, DATABASES, AND DECISION MAKING

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## A Common View of Information Technology

22

## Trends in Enterprise Management - Convergence of Commercial and Technical Computing

- **The web browser as a universal interface**
  - *To data, video, instruments, computing*
- **Virtual teams In business and research**
  - *Intranets and collaborative environments*
- **Distributed object architecture**
  - *Java, Activex, CORBA, integrated via the web*
- **Scientific and information visualization**
  - *Data mining petabyte archives*
- **Microprocessor market convergence**
  - *NT/Intel challenging UNIX/RISC*

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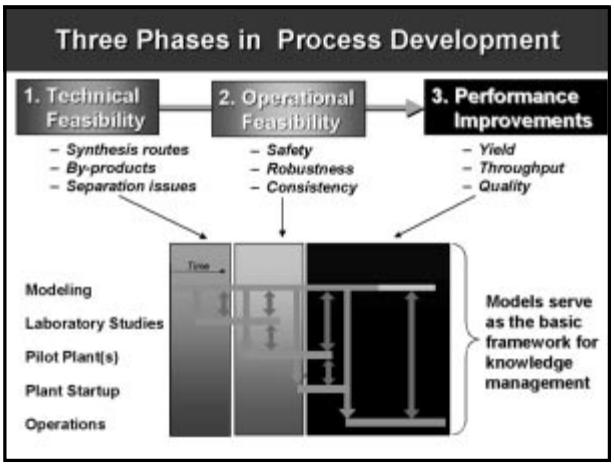
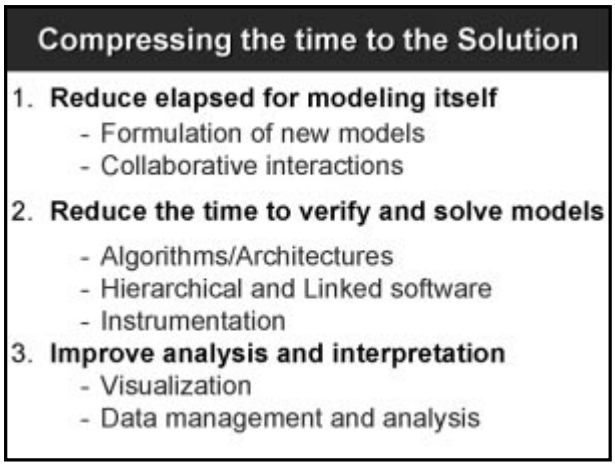
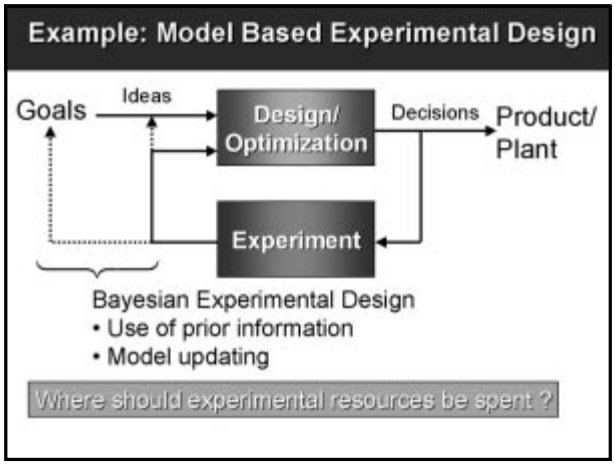



24

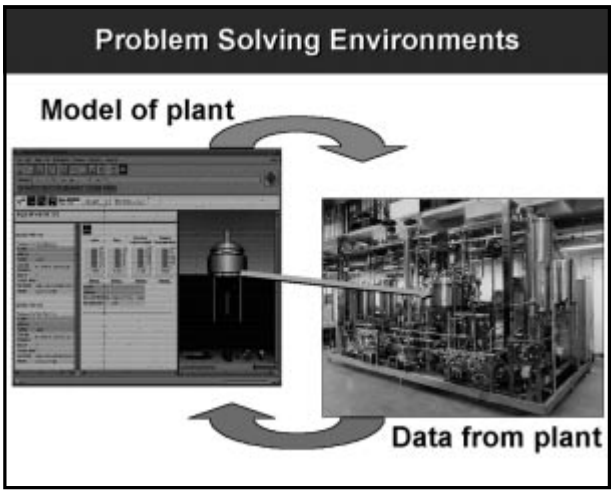
27



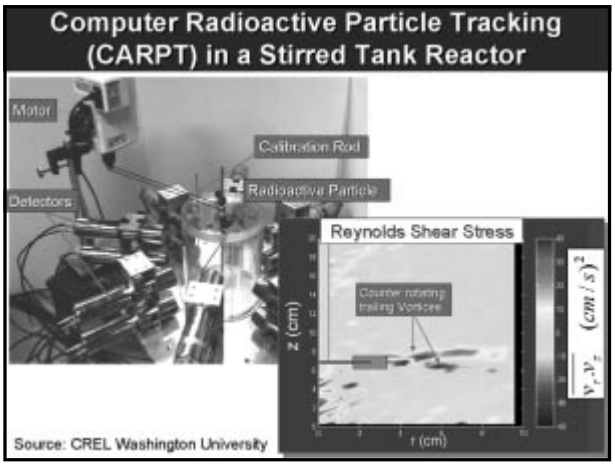

25



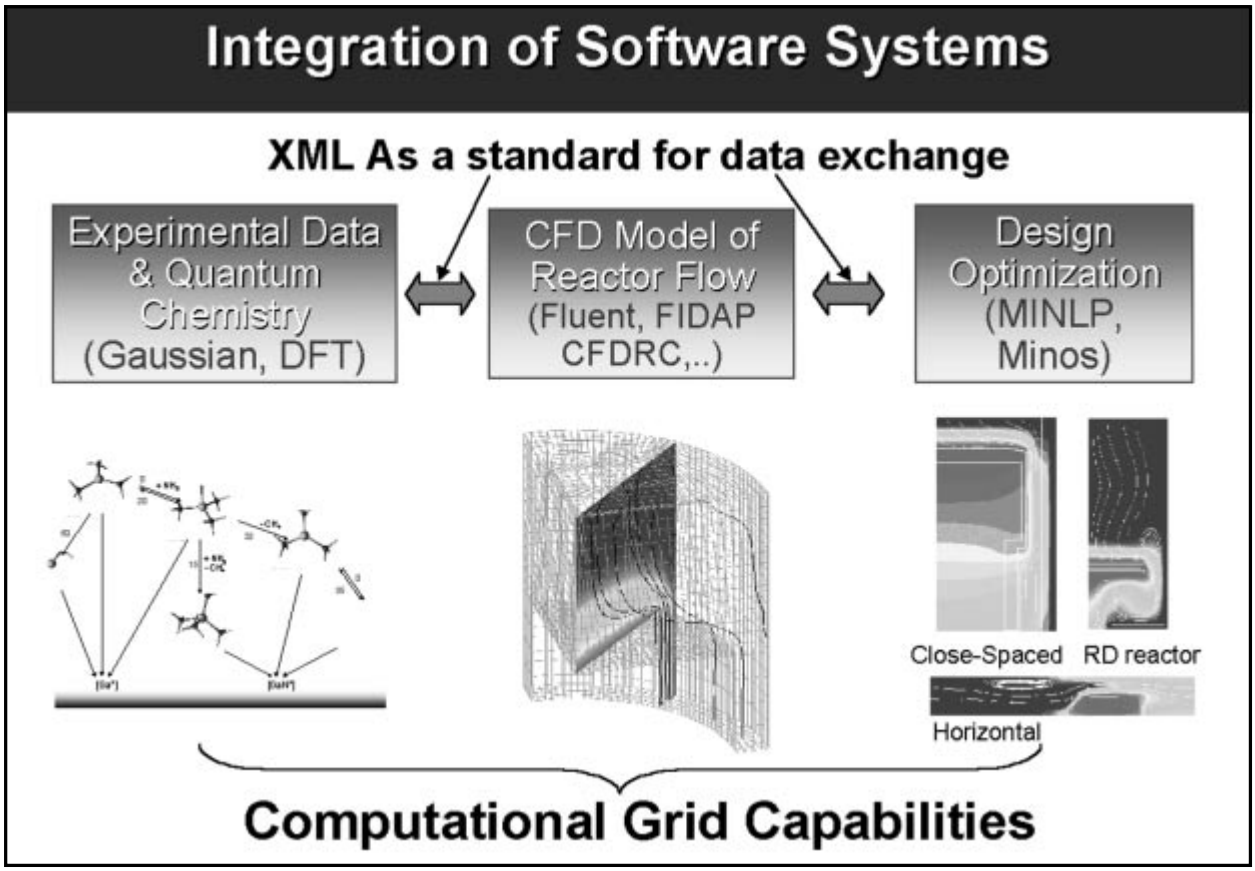

28




26




29


Integration of Software Systems
XML As a standard for data exchange
Experimental Data & Quantum Chemistry (Gaussian, DFT)
CFD Model of Reactor Flow (Fluent, FIDAP CFDRC,..)
Design Optimization (MINLP, Minos)
Close-Spaced
RD reactor
Horizontal
Computational Grid Capabilities

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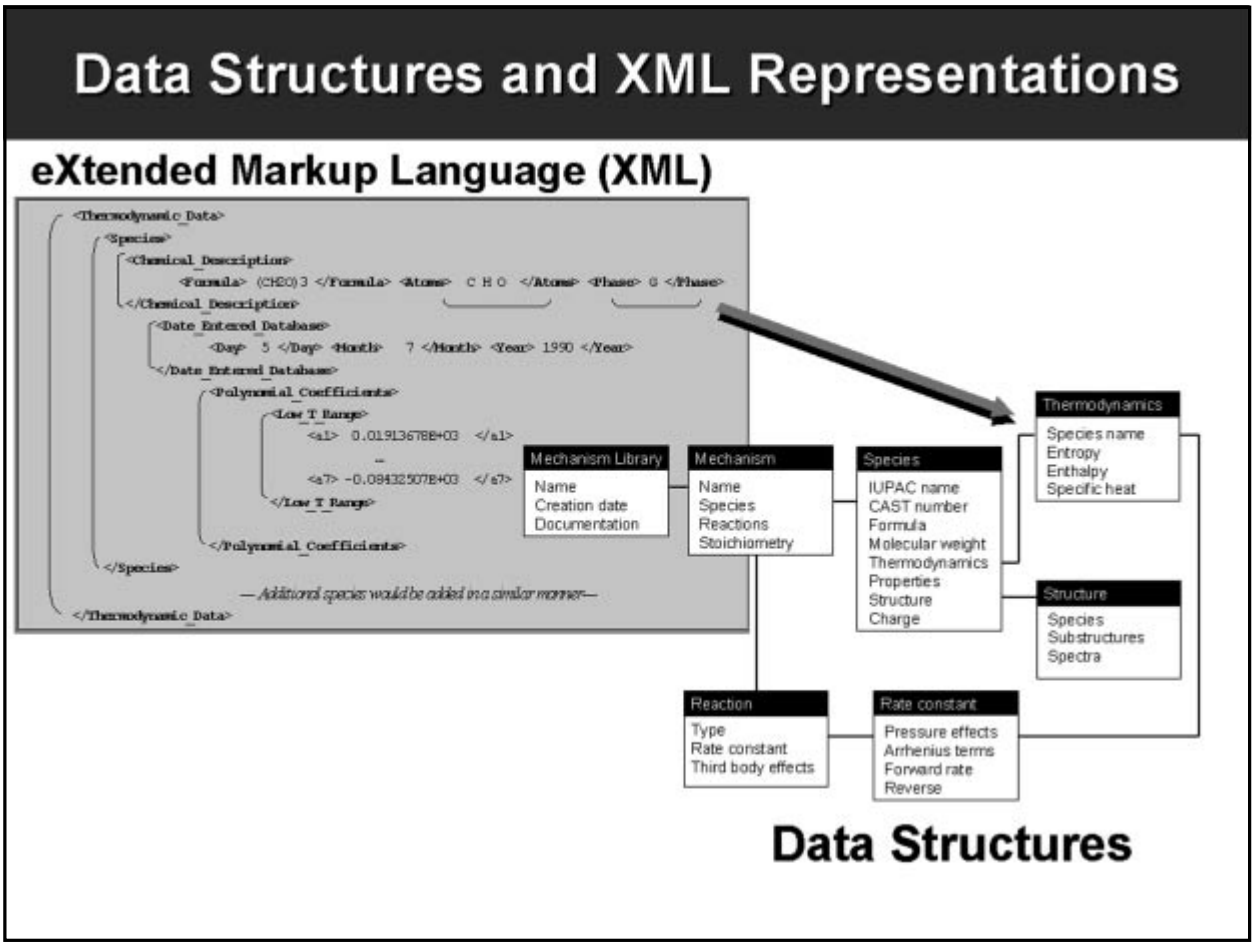
Data Structures and XML Representations
eXtended Markup Language (XML)
<Thermodynamic_Data>
<Species>
<Chemical_Description>
<Formula> (CH2O)3 </Formula> <Atoms> C H O </Atoms> <Phase> G </Phase>
</Chemical_Description>
<Date_Entered_Database>
<Day> 5 </Day> <Month> 7 </Month> <Year> 1990 </Year>
</Date_Entered_Database>
<Polynomial_Coefficients>
<Low_T_Range>
<a1> 0.01913678E+03 </a1>
<a7> -0.09432507E+03 </a7>
</Low_T_Range>
</Polynomial_Coefficients>
</Species>
— Additional species would be added in a similar manner —
</Thermodynamic_Data>
Mechanism Library
Name
Creation date
Documentation
Mechanism
Name
Species
Reactions
Stoichiometry
Species
IUPAC name
CAST number
Formula
Molecular weight
Thermodynamics
Properties
Structure
Charge
Thermodynamics
Species name
Entropy
Enthalpy
Specific heat
Structure
Species
Substructures
Spectra
Reaction
Type
Rate constant
Third body effects
Rate constant
Pressure effects
Arrhenius terms
Forward rate
Reverse
Data Structures

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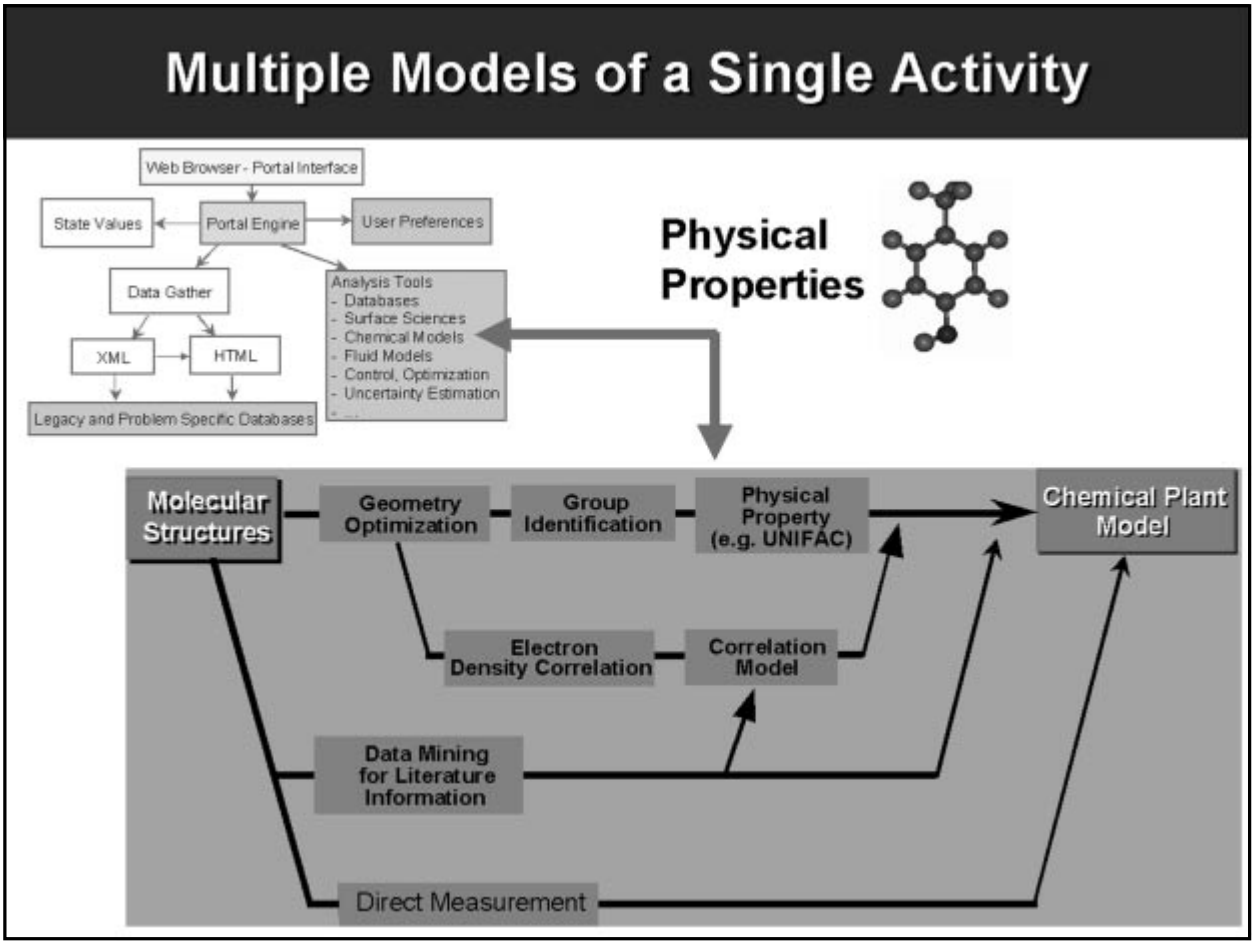
Multiple Models of a Single Activity
Web Browser - Portal Interface
State Values
Portal Engine
User Preferences
Data Gather
Analysis Tools
- Databases
- Surface Sciences
- Chemical Models
- Fluid Models
- Control, Optimization
- Uncertainty Estimation
XML
HTML
Legacy and Problem Specific Databases
Physical Properties
Molecular Structures
Geometry Optimization
Group Identification
Physical Property (e.g. UNIFAC)
Chemical Plant Model
Electron Density Correlation
Correlation Model
Data Mining for Literature Information
Direct Measurement

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AN INTEGRATED APPROACH TO RESOURCE MANAGEMENT:
3. INCORPORATING UNCERTAINTIES INTO THE PRODUCT AND PROCESS DEVELOPMENT CYCLE

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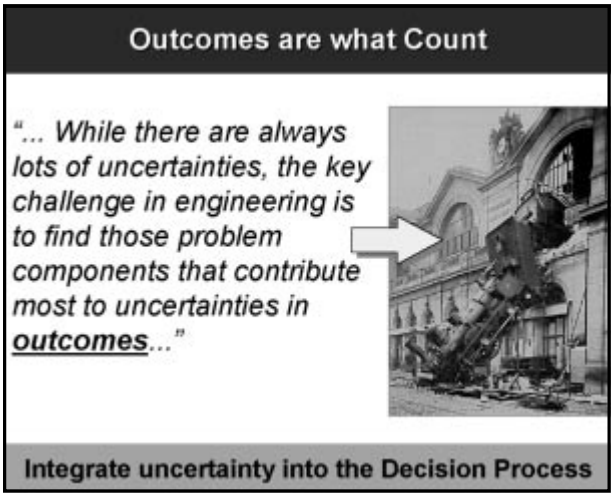
Outcomes are what Count
"... While there are always lots of uncertainties, the key challenge in engineering is to find those problem components that contribute most to uncertainties in outcomes..."
Integrate uncertainty into the Decision Process

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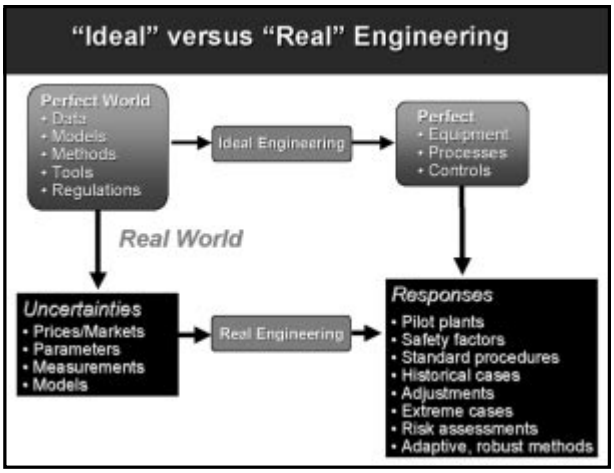
"Ideal" versus "Real" Engineering
Perfect World
• Data
• Models
• Methods
• Tools
• Regulations
Ideal Engineering
Perfect
• Equipment
• Processes
• Controls
Real World
Uncertainties
• Prices/Markets
• Parameters
• Measurements
• Models
Real Engineering
Responses
• Pilot plants
• Safety factors
• Standard procedures
• Historical cases
• Adjustments
• Extreme cases
• Risk assessments
• Adaptive, robust methods

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Uncertainty and Need for Risk Management
• Sales and market forecasts
• Regulatory environment
• Raw material price/availability
• Management/organizational changes
• Stakeholder patience
• Technical assumptions
• Available resource base
• Operational upsets

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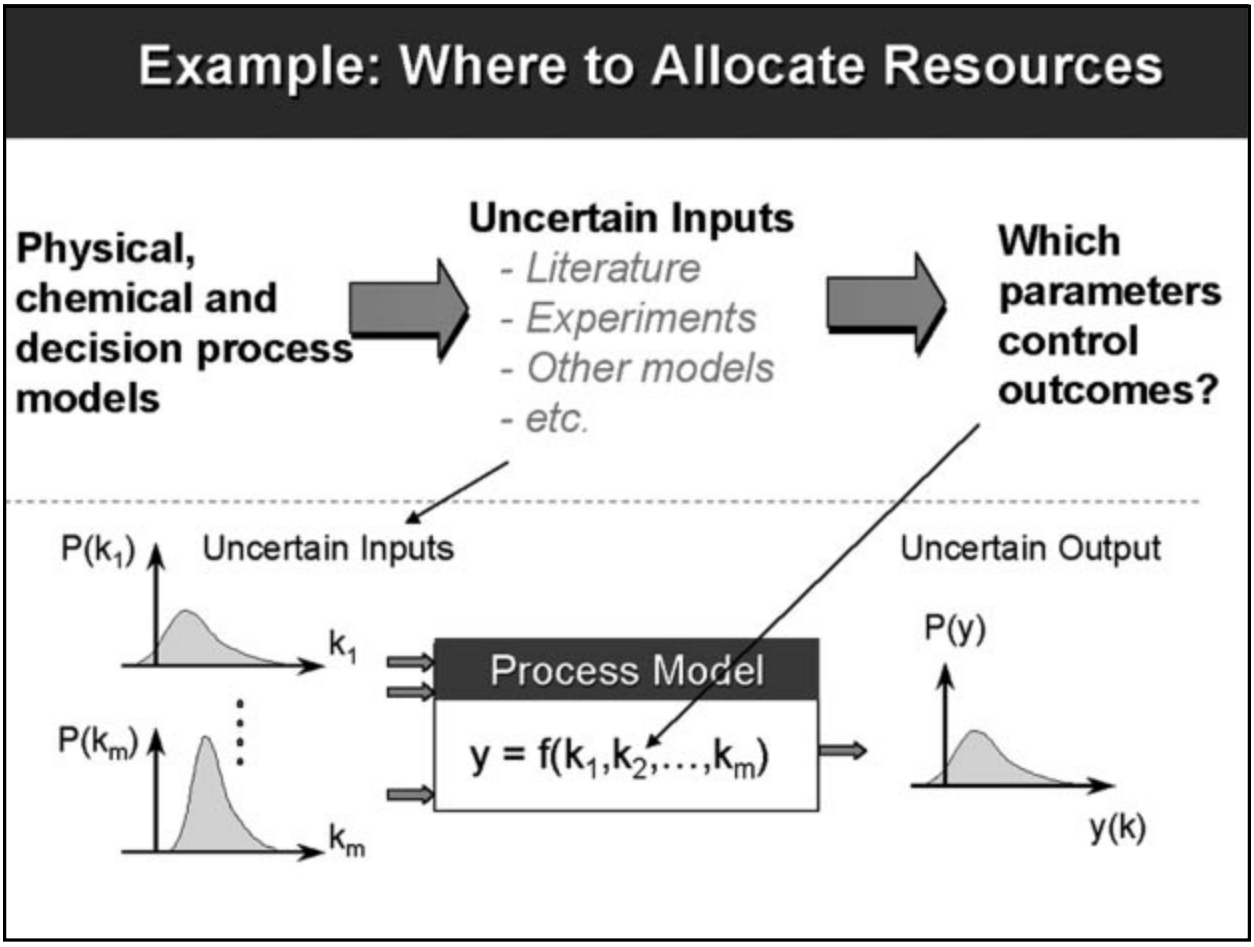
Example: Where to Allocate Resources
Physical, chemical and decision process models
Uncertain Inputs
- Literature
- Experiments
- Other models
- etc.
Which parameters control outcomes?
P(k1)
Uncertain Inputs
k1
P(km)
km
Process Model
y = f(k1,k2,…,km)
Uncertain Output
P(y)
y(k)

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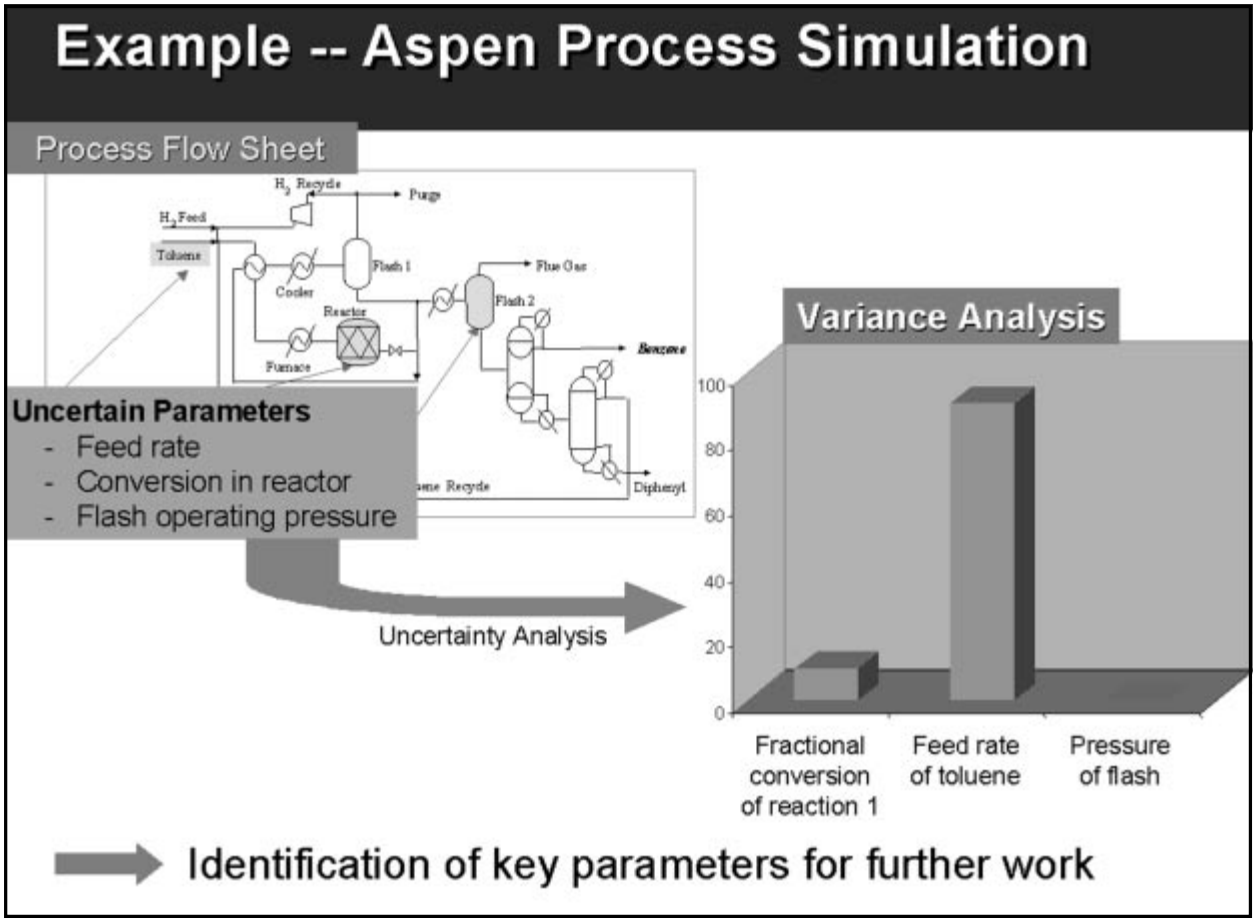
Example -- Aspen Process Simulation
Process Flow Sheet
Purge
Toluene
Flash 1
Flue Gas
Cooler
Reactor
Flash 2
Furnace
Benzene
Diphenyl
Uncertain Parameters
- Feed rate
- Conversion in reactor
- Flash operating pressure
Uncertainty Analysis
Variance Analysis
100
80
60
40
20
0
Fractional conversion of reaction 1
Feed rate of toluene
Pressure of flash
Identification of key parameters for further work

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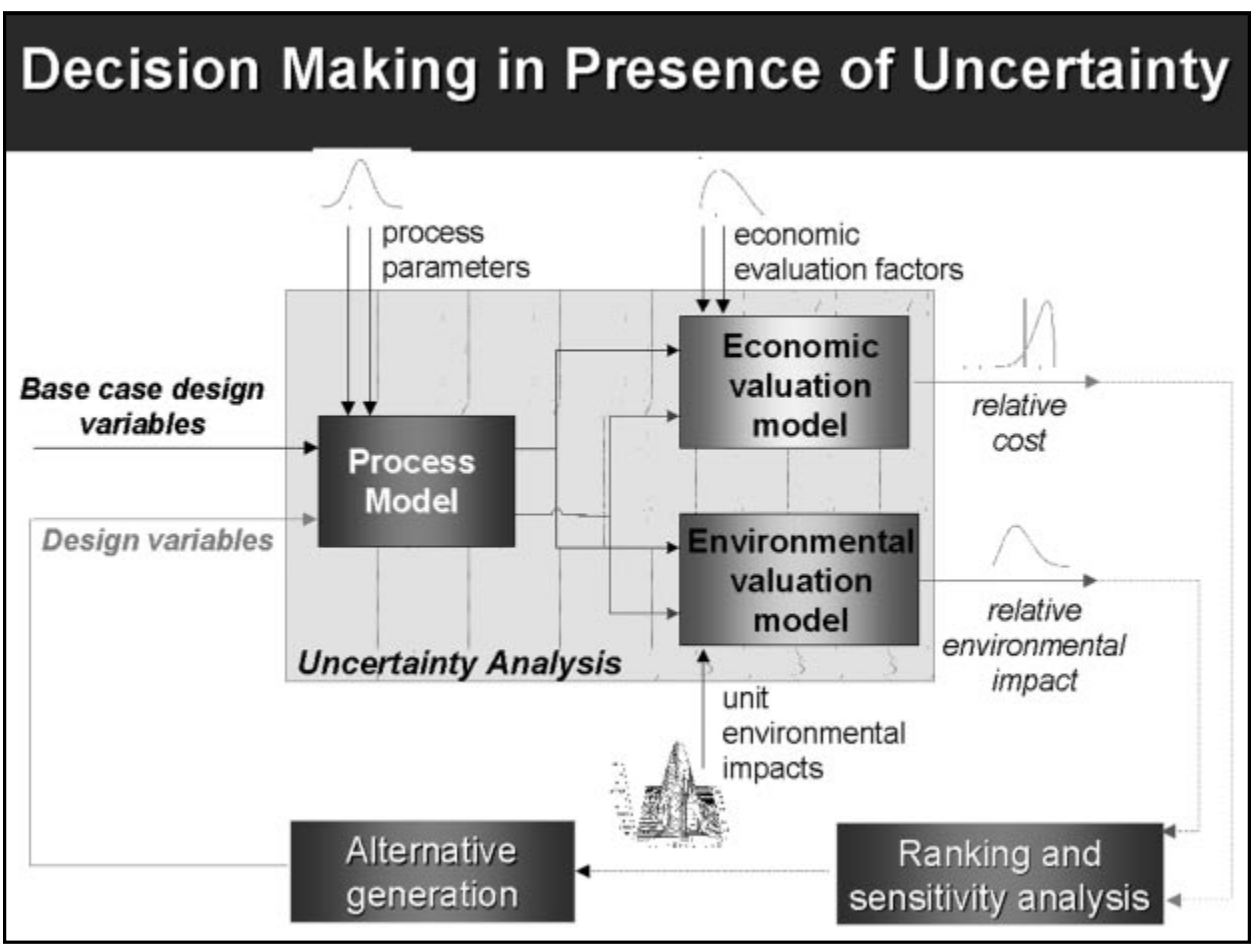
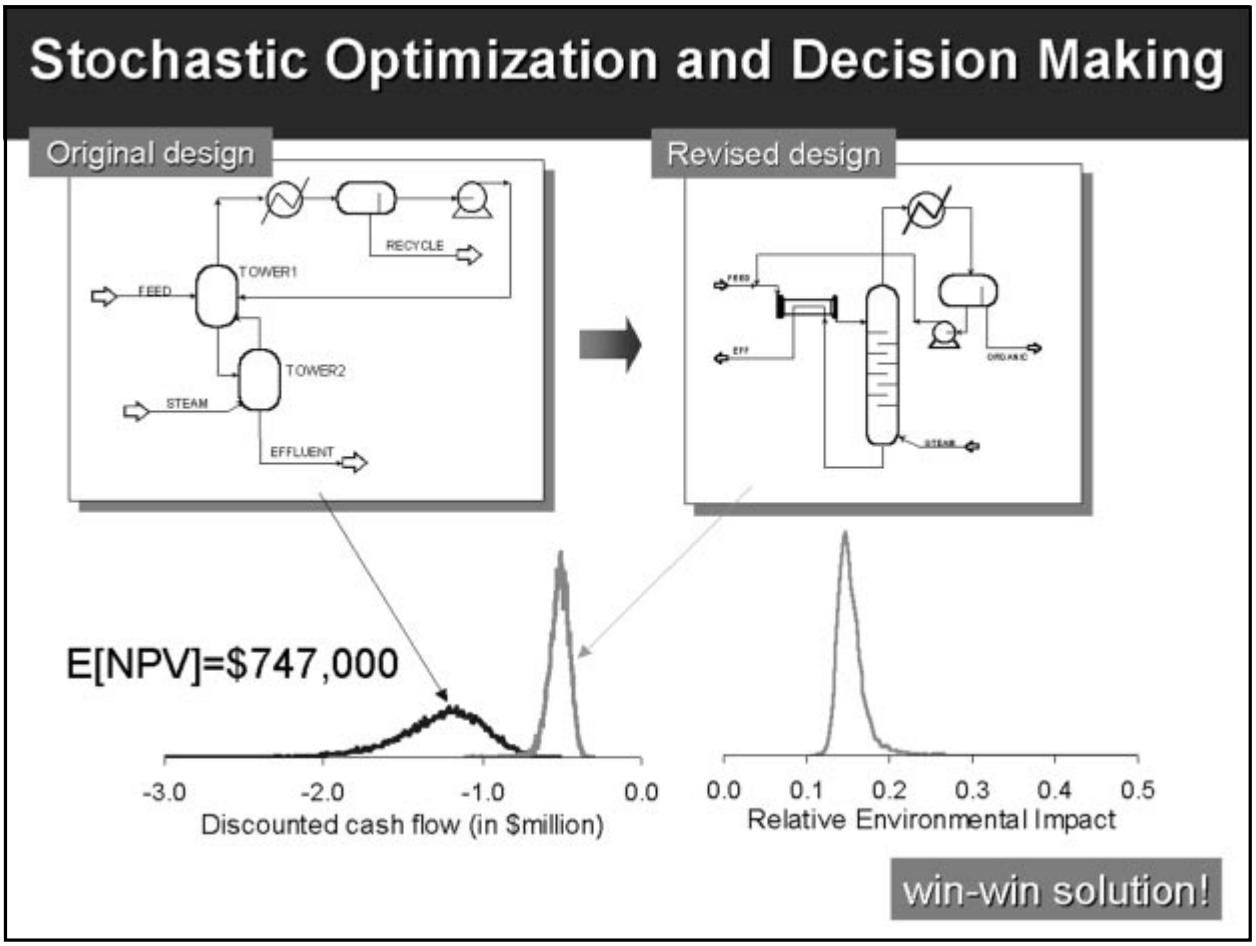

Decision Making in Presence of Uncertainty
process parameters
economic evaluation factors
Base case design variables
Process Model
Design variables
Economic valuation model
Environmental valuation model
Uncertainty Analysis
relative cost
relative environmental impact
unit environmental impacts
Alternative generation
Ranking and sensitivity analysis

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## Vision 2020 – Conclusions/Questions

1. Why settle for just 30% improvements?
2. What are the "real" barriers to reducing the time to market?
3. How to establish standards for representing information/knowledge?
4. What are the educational implications?
5. How to represent uncertainties?

"…it is hard to predict the future, creating it is much easier..."

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