Annual Report
Fiscal Year 2001

Office of Industrial Technologies
Chemical Industry of the Future

Energy Efficiency and Renewable Energy
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Introduction

Industry consumes 36 percent of all energy used in the United States. By developing and adopting more energy-efficient technologies, U.S. industry can boost its productivity and competitiveness while strengthening national energy security, improving the environment, and reducing emissions linked to global climate change.

The U.S. Department of Energy's (DOE) Office of Industrial Technologies (OIT) works in partnership with U.S. industry to increase the efficiency of energy and materials use, both now and in the future. Through an innovative, industry-driven strategy known as Industries of the Future (IOF), OIT helps industry develop and apply advanced, energy-efficient technologies. The strategy maximizes the energy and environmental benefits of OIT's technology investments by forming collaborative partnerships with nine energy-intensive industries:

- Agriculture
- Aluminum
- Chemicals
- Forest Products
- Glass
- Metal Casting
- Mining
- Petroleum
- Steel

Collectively, these streamlined, technology-intensive industries produce $1 trillion in annual shipments, account for 5 percent of the GDP, and supply more than 90 percent of the materials used in our finished products. The materials they produce are vital to our growing high-tech economy.

Chemical Industry of the Future (IOF)

The U.S. chemical industry is the world's largest, accounting for 25% of world chemical production. Chemicals are the building blocks of many products that meet our most fundamental needs for food, shelter, and health, and support such advanced technologies as computing, telecommunications, and biotechnology. The industry produced annual shipments valued at $460 billion in 2000 and generated a trade surplus of over $6.2 billion.

Energy is essential to the chemical industry both as a source of heat and power for plant operations and as a raw material. While the U.S. chemical industry has significantly improved its energy efficiency over the past several decades, it still consumes 6.7 quadrillion Btu's (quads) per year, or close to 25 percent of all U.S. manufacturing net energy use.

Collaboration for competitiveness

Through the IOF strategy, OIT has established formal partnerships with nine energy-intensive industries. Each of these industries has developed a broad "vision" of its future and one or more roadmaps reflecting industry consensus on R&D priorities and other activities needed to achieve its vision. The strategy has also generated:

- Alignment of public-private investment with industry's R&D priorities
- Over 100 commercially successful technologies
- Better industry access to federal laboratory facilities
- Streamlined contracting processes for industry partners
- New industry associations to facilitate and administer collaborative R&D

Chemical industry growth is critically important to the U.S. economy, and technology advances propel that growth. Since chemicals serve as an enabling technology in many other industries, the benefits of chemical research tend to ripple through the economy. The public spillover benefits of research and development (R&D) investments are greatest for basic research because the new knowledge may be used by researchers in other organizations or in government or university labs. Today, most company-funded R&D investments, however, favor relatively short-term product development over basic or applied R&D on the enabling technologies needed to grow the industry. To leverage available resources, R&D partnerships among government, industry, and academia are essential to maintaining the industry's competitive edge in a rapidly expanding global market.

OIT's IOF strategy fosters collaborative public-private R&D partnerships. By participating in IOF partnerships, the chemical industry is pursuing innovative technology development that ensures future competitiveness and sustainable growth.

The chemical industry is reaping multiple benefits from this partnership:

- Clearly defined R&D goals and pathways to their successful attainment
- A powerful common voice to guide government investment
- Expanded resources to accelerate R&D
- Multi-disciplinary approaches to industry needs
- Cleaner, more energy-efficient technologies and processes, including use of alternative feedstocks
- Increased plant productivity and profitability now and in the future

Benefits to local communities and the nation

- Cleaner air
- Decreased greenhouse gas emissions
- Enhanced quality of food, health, housing, and transportation
- Improved energy security
- Conservation of energy and natural resources

The Chemical IOF enjoyed a landmark year in fiscal year (FY) 2001. The partnership has continued to build upon an already robust portfolio of cost-shared R&D projects that tackle some of the industry's toughest technological challenges. The diverse R&D partners are breaking new ground in process science and engineering technology, chemical synthesis, computational technologies, materials technology, and bioprocesses and biotechnology. The results of these projects promise to boost energy efficiency and productivity in a broad spectrum of chemical industry sectors over the near-, mid-, and long-term. In addition, the industry has gained improved access to a wide range of tools and resources for improving energy efficiency and productivity today, particularly through the IOF BestPractices program. This program offers plant-wide assessments, energy management tools, and informative publications to help provide rapid solutions to present problems.

The Chemical IOF is also benefiting from the emergence of the Chemical Industry Vision2020 Technology Partnership (Vision2020) — a collaboration of U.S. chemical companies dedicated to accelerating innovation and technology development. With the establishment of Vision2020, the chemical industry now has a leadership organization to leverage resources and provide a unified voice to guide public and private R&D investment. Vision2020 is helping to guide development of the Chemical IOF R&D portfolio and encouraging diverse sectors of the chemical industry to participate in the development and deployment of technologies and innovations that will benefit the industry and the Nation.

This Annual Report for 2001 highlights the many activities of the Chemical IOF. The next section, Chemical IOF Strategy, provides an overview of achievements in 2001. The Chemical Industry Trends and Drivers section identifies the issues affecting the R&D portfolio development process. The section on Chemical IOF Highlights identifies how the Chemical IOF is accelerating R&D and technology implementation by building partnerships and developing tools for industry. 2000-2001 R&D Progress and Successes provides a profile of new technology development projects co-funded by OIT. Active R&D projects are described in the 2001 Chemical IOF R&D Portfolio.

Chemical IOF Strategy

Today, U.S. industries face serious energy, economic, and environmental challenges that affect their domestic and international competitiveness. OIT strives to help industry meet these challenges by developing and deploying technologies that increase energy efficiency, reduce waste, improve productivity, and enhance environmental performance. Through OIT's IOF process, public-private partnerships share the risks and costs of technology R&D. The industry-led process ensures that activities yield the greatest possible benefit to the industry while achieving national goals for energy and the environment.

Vision and Roadmaps

To guide technology development for the chemical industry, over 300 chemical companies and associations collaborated on the development of the *Technology Vision 2020: The U.S. Chemical Industry*. This landmark document, released in 1996, outlines a unified vision for the chemical industry in 2020. The document identifies industry-wide goals for making more efficient use of energy and raw materials, better managing of the supply chain, and enhancing environmental performance for a more profitable and sustainable future.

The Vision document set broad goals for future R&D in four critical areas: New Chemical Science and Engineering Technology, Supply Chain Management, Information Systems, and Manufacturing and Operations. Groups of chemical companies have come together to jointly develop R&D agendas or "roadmaps" that outline priority R&D needs and performance targets within critical technology areas. To date the industry has completed roadmaps for the following nine areas:

Chemical Industry
VISION 2020
Technology Partnership

An industry-led process to accelerate innovation and technology development by leveraging financial and technical resources www.chemicalvision2020.org.

Biocatalysis, Combinatorial Chemistry, Computational Chemistry, Computational Fluid Dynamics, Materials of Construction, Materials Technology, New Process Chemistry, Reaction Engineering, and Separations. To achieve the Vision goals and technology performance targets defined in these roadmaps, the U.S. chemical industry is leveraging its R&D resources by working with OIT as a part of the Chemical IOF strategy.

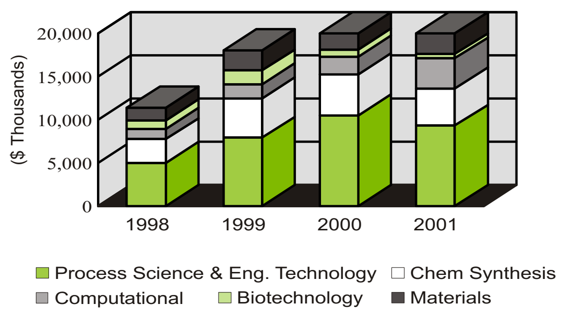
Vision2020 Technology Partnership

In 1999, an informal group of senior chemical industry leaders helped guide the Chemical IOF effort and explored new strategic directions for the industry. This informal group, called the Chemical Industry Executive Steering Group (CIESG), organized a "Vision2020: Next Steps" workshop in September 2000 to update and reinvigorate the industry's vision and roadmapping initiative. Participants formalized plans for a new, broad-based organization to lead the chemical industry's R&D efforts. The resulting organization, Vision2020, now represents the industry side of the Chemical IOF effort. It plays an integral role in the overall IOF process, leveraging resources and guiding development of critical enabling technologies for chemical processing.

Portfolio of R&D Projects

To further the goals of the Chemical IOF, OIT provides cost-shared funding for R&D projects that respond to one or more roadmap priorities and also provide energy and environmental benefits. All R&D awards are based on a competitive solicitation process open to collaborative teams that draw members from industry, national laboratories, academia, and other sectors with a stake in the future of the U.S. chemical industry. Through this cost-shared funding, the Chemical IOF fosters the development of R&D partnerships that will ultimately increase the efficiency of energy-intensive processes used in large-commodity chemical production. Since 1998, OIT has provided over $48 million in cost-shared support for collaborative R&D projects (see Figure 1.). Through these collaborative R&D partnerships, the Chemical IOF has built a robust portfolio of projects that will help meet national energy and environmental goals and give industry an edge in global markets. R&D projects currently funded directly through OIT's Chemical IOF will have a total project cost of about $105 million (through the duration of all projects). OIT will be providing about $53 million and the total industry cost share will amount to over $52 million.

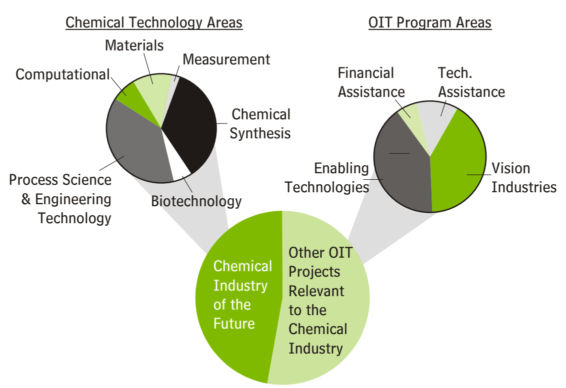
Figure 1. Chemical IOF Federal R&D Investment Portfolio Aligned with Vision2020 Priorities*



* Total investment includes DOE/SBIR funding.

The Chemical IOF also benefits from the resources and activities of other parts of the IOF partnership (see Figure 2.). Collectively, the other eight energy-intensive industries participating in the IOF strategy are pursuing over 20 R&D projects relevant to the chemical industry. Through OIT's crosscutting programs, R&D is underway to improve sensors and controls, combustion, and materials that can benefit the chemical industry. In addition, the Chemical and Petroleum IOFs are working together to implement activities in Texas and many other states through state-level IOF efforts, and chemical companies such as Akzo Nobel, 3M, Bayer Corporation, W.R. Grace, Neville Chemical, and

Figure 2. OIT Chemical R&D Portfolio
Number of Projects FY 2001: 78



Rohm and Haas are taking advantage of the plant-wide assessments offered through the IOF BestPractices effort.

Get Involved with the Chemical IOF

Requests for Proposals (RFP) are available on the OIT Web site at www.oit.doe.gov/chemicals, along with more information on OIT activities. To discover more about the latest resources to improve energy efficiency, call OIT's Clearinghouse at 1-800-862-2086. For more information on Vision2020 opportunities, visit the Web site at www.ChemicalVision2020.org.

Chemical Industry Trends and Drivers

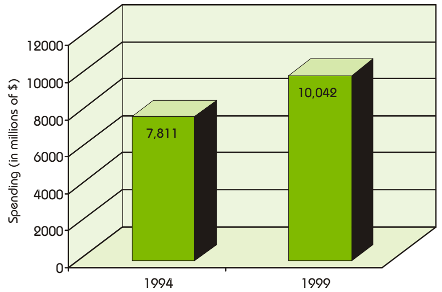
The Chemical IOF strategy emphasizes industry leadership. In addition to preparing the vision and roadmaps, the industry plays an active role in shaping OIT's R&D portfolio and other industry-related activities. With the establishment of Vision2020 the chemical industry has gained an even stronger voice in public-private R&D investments. The industry's challenges and priority needs continue to drive the Chemical IOF process.

Industry Snapshot

The U.S. chemical industry is a leader in the global marketplace and has experienced substantial growth over the past decade. With annual shipments valued at more than $460 billion in 2000, it is the world's largest chemical producer. Chemical industry growth and sustainability are vitally important to the nation's economy. The industry contributes 2.1% of the annual U.S. GDP and is a large net exporter of products, with a trade surplus of over $6 billion in 2000. The industry directly employs over a million people, and approximately 36 million more people work in businesses that rely on chemicals. The primary markets of the U.S. chemical industry are U.S. manufacturing industries, including automotive, construction, and commodity materials such as glass and paper.*

The chemical industry is a dynamic, internationally competitive industry that invests billions of dollars annually in R&D and relies on advanced technology to capture market share (see Figure 3.). Energy efficiency is also important to the industry, which uses fossil fuels for both fuel and feedstock. The chemical industry consumes 6.7 quads per year (approximately 25% of all net energy used by U.S. manufacturers).

Figure 3. Total R&D Spending by the Chemical Industry



Not only are chemicals essential to many products and consumer goods, but chemicals also enable numerous technological advances. During the past ten years, the chemical industry has diversified, increasing its presence in high technology areas such as advanced materials, biotechnologies, and pharmaceuticals. Along with this diversification has come an increase in R&D spending, with the majority of investment directed at product development. A recent study sponsored by the Council for Chemical Research (CCR) pointed out the trickle-down benefits of chemical research in many industries and highlighted the need for a broad domestic science base to spur technological development and innovation.**

Updating Industry Needs

As the U.S. chemical industry looks to the future, it faces tough economic, energy, and environmental challenges. Factors such as globalization, rising energy costs, and increasing environmental regulations play crucial roles in the industry's growth. The industry has come to recognize that its future growth and competitive advantage will depend upon the collaborative efforts of industry, government, and academia. Vision2020 is seeking to unite the chemical industry and to leverage and redirect public investment toward basic enabling R&D projects that are beyond the risk and payback horizon of individual companies.

At OIT's biennial Expo held in February 2001, Vision2020 hosted a roundtable of chief technology officers (CTOs) and other chemical industry leaders to elicit their views on the problems, solutions, and opportunities facing the industry. Technology leaders from Air Products and Chemicals, BP, Dow Chemical, DuPont, Equistar, General Electric, and Praxair played active roles in the discussion. Meeting sponsors included the American Chemical Society (ACS), the American Institute of Chemical Engineers (AIChE), CCR, and OIT. Roundtable participants enumerated the major barriers facing their own companies, and suggested R&D projects that could accelerate growth industry-wide.

*Bureau of the Census, Bureau of Labor Statistics, Bureau of Economic Analysis, and the American Chemistry Council

***Measuring Up: Research and Development Counts for the Chemical Industry,* The Council for Chemical Research in cooperation with The Chemical Heritage Foundation, 2001.

Roundtable participants concluded that the chemical industry needs new enabling technologies to build the foundation for market-level innovation and partnerships among companies to leverage resources. The willingness of chemical companies to collaborate marks a major milestone for this fiercely competitive industry.

Technology leaders from leading chemical companies attended the Chemical CTO Roundtable in February 2001.

Key Needs

Need: Enabling technologies that produce sustainable industry growth. The chemical industry is currently faced with the task of developing more environmentally friendly and energy-efficient technologies, while simultaneously continuing to achieve growth in an increasingly globalized market. Development of basic enabling technologies can help the industry achieve future growth and profitability as well as long-term sustainability. Technology advances should respond to related issues such as capital intensiveness, performance and safety standards, management of NO_x and greenhouse gases, waste reduction, and energy and water consumption.

Need: Revolutionary partnerships to accelerate technology breakthroughs. A collaborative approach can help pave the way to faster, smarter R&D. Fostering new R&D communities and establishing ways to leverage public expertise, facilities, and investments will help the industry accelerate innovation and technological advances. To identify the R&D most suitable for collaborative projects, industry must develop a better understanding of long-term, industry-wide technology needs and trends. Other issues to be addressed include developing ways to measure the success of R&D efforts (e.g., impacts, intellectual property), revitalizing R&D at the university level, and increasing integration among suppliers.

Pre-Competitive Areas for Collaborative R&D:

- New chemistry to improve conversion rates
  - Synthesis
  - Catalysis
- Better, more flexible processes
  - Revolutionary separations
  - Replacements for crystallization and distillation
  - Biotechnology
- E-business for enhanced flexibility
  - Generic information exchange
  - Database standards
  - Information technology
  - Business to business
  - Outsourcing services
  - Remote operation
- Dynamic process control
  - Real-time sensors
  - Non-invasive analysis
- Computational technologies to improve material transport
  - Methods and tools
  - Simulation and modeling

Chemical IOF Highlights

The Chemical IOF and the chemical industry have worked closely over the past year on a wide range of activities to benefit chemical producers. These activities include fostering collaborative partnerships, producing new roadmaps, developing useful tools and publications, and helping plants identify opportunities for energy savings. This summary of activities highlights the diverse range of opportunities made available through the Chemical IOF's expanding array of products and services.

Industry-Wide Organization Leads Chemical IOF

The establishment of Vision2020 represents an important milestone in the development of the Chemical IOF. For the first time, an industry organization represents the needs of the entire chemical industry, bridging diverse interests and creating a unified voice. Vision2020 provides the Chemical IOF with a more focused industrial partnership effort and increased potential for industry-wide implementation of OIT projects. The organization will play an active role in shaping the Chemical IOF portfolio by recommending technical areas for solicitations and providing technical evaluation of proposals and ongoing R&D projects.

The informal group that initially guided the Chemical IOF effort, CIESG, officially passed the torch to Vision2020 in September 2001. The newly established Vision2020 is composed of leading chemical companies that have pledged their time and resources to the partnership. Each member company will contribute $5,000 per year to cover organization operation costs.

Chemical companies who have joined the Vision2020 Steering Committee as of September 1, 2001:

- Air Products and Chemicals, Inc.
- BP
- Cargill Incorporated
- Ciba Specialty Chemicals
- Degussa Corporation
- The Dow Chemical Company
- Dow Corning Corporation
- E.I. du Pont de Nemours and Company
- General Electric Company
- Millenium Chemicals
- Praxair, Inc.
- Rohm and Haas Company

In addition, the following organizations are participating in the Vision2020 Technology Partnership:

- American Chemical Society
- Council for Chemical Research
- American Institute of Chemical Engineers
- Materials Technology Institute

Partnerships Pursue Priorities

Partnering is a strategy that is catching on throughout industry. Corporations around the globe are joining forces and leveraging resources to accelerate progress toward common goals. Within the U.S. chemical industry, the completed chemical technology roadmaps have provided a powerful stimulus for collaboration, launching numerous new partnerships. Partnerships of special significance to the U.S. chemical industry are the Multi-Phase Fluid Dynamics Research Consortium (MFDRC) and OIT's collaborations with MTI, AIChE, and the Texas State IOF.

The Multi-Phase Fluid Dynamics Research Consortium

MFDRC was formed in 1998 in response to priority research needs identified in the *Computational Fluid Dynamics Roadmap*. With its current membership of ten companies, seven universities, and five national laboratories, MFDRC is pushing the frontier for the modeling of materials transport. The consortium is using approximately $10 million in funding to undertake a balanced program of fundamental research and technology development in order to better understand and model multi-phase flows. Partners plan to develop commercial software packages using the more accurate, reliable, and cost-effective computational modeling tools, which will help solve common production problems throughout the chemical industry. For additional information, visit the MFDRC Web page at http://www.mfdrc.org.

Materials Technology Institute Collaboration

MTI's collaboration with OIT has led to five new industry partnerships that address priorities identified in the *Materials of Construction Roadmap*. Corrosion and other material failures cost the chemical industry billions of dollars each year. Advanced materials will yield significant payoffs in plant energy efficiency and overall plant safety. Companies and MTI will contribute $8.4 million in addition to technical expertise and test sites, while Oak Ridge National Laboratory, Argonne National Laboratory, and other selected industrial partners conduct the R&D. The partners are leveraging approximately $6 million from DOE over the life-span of the projects. Descriptions of the five projects sponsored through MTI partnerships appear under the Materials heading in the 2001 Chemical IOF R&D Portfolio section of this report.

AIChE and FMC Become Allied Partners

AIChE announced its participation as an Allied Partner of OIT at the OIT Expo in February 2000. While AIChE already supports its industry members with products, services, and forums to help meet energy efficiency challenges, the Allied Partnership will provide industry with an even larger suite of tools and programs. As part of the Allied Partner Agreement, AIChE will promote OIT's extensive portfolio of energy efficiency products and services to a broad spectrum of energy-intensive industries through AIChE's Operational Excellence program. The Allied Partnership will allow AIChE and OIT to leverage their respective efforts by promoting awareness of OIT programs to the more than 55,000 AIChE members. OIT and AIChE will exchange information on energy efficiency through AIChE's journal *Chemical Engineering Progress*, AIChE technical products, AIChE and OIT Web sites, and training and seminars at AIChE national meetings and local section functions. For more information, visit the AIChE Web page at www.aiche.org or the Allied Partners Web page at www.oit.doe.gov/bestpractices/meet_partners.

FMC Corporation is one of the world's largest producers of chemicals for industry and agriculture. The company's Chemical Products Group (CPG), which originally learned of OIT's Allied Partnership opportunities through the *Energy Matters* newsletter, officially came onboard as an Allied Partner in August 2001. CPG is composed of three wholly owned, U.S.-based divisions: Alkali Chemicals Division (producer of natural soda ash), Hydrogen Peroxide Division, and Active Oxidants Division.

As part of FMC's company-wide initiative to improve resource efficiency, CPG has formed site energy reduction teams and interdivisional energy-focused technology support teams. As an Allied Partner, CPG is applying OIT products, tools, and services in-house and is promoting the use of OIT's energy-efficiency tools and strategies within the industry. The FMC/CPG Allied Partnership with OIT will focus on the following initiatives:

- Raising awareness of and disseminating OIT information and resources
- Conducting energy assessments
- Providing training workshops on energy efficiency
- Participating in Texas Industries of the Future activities
- Evaluating opportunities to implement emerging technologies

Texas State IOF Fosters R&D

The Texas State IOF is becoming increasingly involved with Chemical IOF activities. The Texas economy relies on the chemical industry for a large portion of its value chain. Texas employs more than 80,000 chemical industry workers in its more than 1,000 facilities. While the industrial sector accounts for over 50% of the energy usage in Texas, the chemical industry consumes over 40% of that energy.

The Chemical IOF, in collaboration with State IOF activities, will help facilitate development, demonstration, and adoption of advanced technologies in Texas to reduce industrial energy usage, emissions, and their associated costs. Planned activities this year include a workshop on low NO_x combustion technology and energy efficiency strategies, a workshop to review national technology roadmapping efforts and identify needs specific to Texas, and other opportunities to learn about federal funding availability. For more information about the Texas State IOF, visit the Texas IOF Web page at http://texasiof.ces.utexas.edu.

New Roadmaps

The Chemical IOF supported the chemical industry to complete new roadmaps for Combinatorial Chemistry, Materials Technology, Biocatalysis, Separations, Reaction Engineering, and New Process Chemistry in 2000 and 2001. Each roadmap is a strategic plan that identifies priority research needs for a specific technology area of critical importance to the chemical industry.

- Combinatorial methods facilitate the discovery of new materials, optimize processes for manufacturing these new materials, and support advances in chemical science and engineering, including chemical synthesis and the development of new catalysts and reaction systems. The *Technology Roadmap for Combinatorial Methods* identifies current capabilities and trends in combinatorial chemistry. It also assesses market drivers, key applications and future themes and goals.

- The *Materials Technology Roadmap* focuses primarily on polymers and supports the Materials Technology area of New Chemical Science and Engineering Technology of Vision 2020. The key challenges for materials technology include prediction of materials properties, synthesis technology for precise manipulation of material structures, enhanced performance in materials, developing routes for step change improvements in performance of materials systems with the use of new additive technology, and developing technology in integrated materials and processes for reuse and disassembly.

- Bioprocesses promise to be exceptionally important in the coming decade, particularly with the development of more energy-efficient and environmentally friendly processes. The *Biocatalysis Roadmap* describes research in protein engineering, biometry, combinatorial chemistry, and related areas.

- Four workshops contributed to the development of the *Separations 2000 Roadmap*. Over 230 experts from chemical and related industries, universities, and government research laboratories participated. These roadmapping activities established a central goal for separations R&D: a 30% reduction in material usage, energy usage, water consumption, toxic dispersion, and pollutant dispersion.

- The *Reaction Engineering Roadmap* identifies technology development needs in reactor design and scale-up, chemical mechanisms, catalysts, and new reactor development. Addressing these research needs should result in optimized, integrated reactor systems with higher selectivity, yield, and purity.

- The *New Process Chemistry Roadmap* focuses on innovative new chemistry to support the technical areas of Process Science and Engineering and Chemical Synthesis. Five workshops were conducted during roadmap development: Dense Phase Fluids and Alternative Reaction Media, the Role of Polymer Research in Green Chemistry and Engineering, Alternative Process Conditions and Electrotechnology, Synthesis and Processing with Alternative Resources, and New Process Chemistry.

New Tools and Publications to Serve You

OIT's Chemical IOF supports the development of a wide range of tools and publications to assist the U.S. chemical industry. A series of metrics tools now under development, and a recent publication with baseline measurements, will be particularly useful to all those engaged in setting quantitative performance targets and measuring progress in chemical processing technology.

New Tools for Setting Efficiency Performance Levels

Metric tools to evaluate energy use in major chemical processes are being developed to help companies benchmark their plants and focus R&D efforts. OIT and the AIChE Center for Waste Reduction Technologies (CWRT) are working together with various chemical users and producers to test and evaluate a subset of sustainability metrics previously formulated by CWRT's Metrics Team for 50 major chemical products as a way to benchmark the processes by which they are made. Another project is underway to determine the feasibility of calculating "practical minimum energy use" for the same set of chemical processes studied in the benchmarking project (see Appendix C). This new project is evaluating three levels of energy consumption: (1) current practice, (2) current best practices, and (3) potential future best energy use considering possible new and future technologies and practices. The initial evaluation phase of the practical minimum energy project has been completed, and the results will be used by AIChE, DOE, and industry to guide future work. Additional information is available on the CWRT Web site at www.aiche.org/cwrt/projects/sustain.htm.

Energy and Environmental Profile Of the Chemical Industry

A publication entitled *Energy and Environmental Profile of the U.S. Chemical Industry* published in May 2000 (see Appendix C) presents an analysis of the impacts of chemical production. The report is an excellent reference for chemical engineers and others working in, selling to, buying from, or otherwise engaged with the chemical industry. It identifies the following chemical production processes that offer the greatest opportunity for reductions in energy use: ethylene, propylene, benzene-toluene-xylene (BTX), agricultural chemicals, chlor-alkali industry, effluent treatment, process heaters, and others. The report supplies the most current estimates of energy use by fuel type for each of the major industry processes. In addition, the report characterizes air emissions, effluents, and other residuals generated by each process, provides estimates of quantities, and describes existing treatment and control technologies. To receive your copy, please call OIT's Clearinghouse at (800) 862-2086.

Plant-Wide Efficiency Assessments

Several U.S. chemical plants have taken advantage of the plant-wide assessments available through OIT's BestPractices program. The results of these assessments are prepared as case studies to help other plants. Most of the activities and technologies are readily applicable in similar industrial environments and should result in similar savings.

Rohm and Haas

The Rohm and Haas Company's facility in Deer Park, Texas, established an energy team in 1996 and has made tremendous energy efficiency improvements. OIT is partnering with Rohm and Haas to continue this progress. The Deer Park plant is the largest monomer manufacturer for key Rohm and Haas products and accounts for 35% of all Rohm and Haas corporate energy use. The chemical monomers produced at this facility form the building blocks for other Rohm and Haas products, so the energy efficiency at the Deer Park plant translates across the entire supply chain, from chemical feedstock to consumer end products. The assessment revealed over 125 ways to reduce energy consumption. To date, the facility has saved a total of $15 million per year and improved overall energy efficiency by 17% on a per-pound-of-chemical-produced basis. In February, the Deer Park facility was named the runner-up for OIT's 2001 Plant-of-the-Year award.

Akzo Nobel

Akzo Nobel, one of the world's largest chemical companies, launched a plant-wide energy efficiency assessment program in November 2000 to reduce energy consumption by 20%. An assessment of their plant in Morris, Illinois, is using process engineering and best practice analysis techniques to evaluate a variety of energy efficiency opportunities in steam systems, electric-motor systems, compressed air systems, heat exchange networks, and combined heat and power systems. OIT is sharing half the assessment costs with Akzo Nobel. Following this pilot assessment, the assessment team will evaluate ten other sites, which account for more than 90% of Akzo Nobel's energy consumption.

Five new plant-wide assessments of chemical company facilities will be co-funded by IOF BestPractices in 2001. These plants include:

- Bayer Corporation in New Martinsville, West Virginia
- Neville Chemical in Anaheim, California
- 3M in Hutchinson, Minnesota
- W.R. Grace in Baltimore, Maryland
- Rohm and Haas in Knoxville, Tennessee

For more information on plant-wide assessments, or any other IOF BestPractices tools, please visit the IOF BestPractices Web site at www.oit.doe.gov/bestpractices.

2000-2001 R&D Progress and Successes

Commercial Successes

The Chemical IOF is committed to helping companies bring innovative new technology into the marketplace. Pre-competitive R&D is often a lengthy and risky process, but some of the Chemical IOF projects are already enjoying commercial success. During 2000, two projects achieved commercial status — a technology to recycle nylon 6 carpet and a technology to recover polyurethane from auto shredder residue. An assortment of additional technologies in the Chemical IOF portfolio should emerge from R&D to become commercialized within the next few years.

Nylon 6 Recycling

A new technology developed by Honeywell (formerly Allied Signal) and DSM Chemicals can help recycle the approximate 1.8 million tons of nylon carpet sent to landfills each year. The technology allows nylon manufacturers to recover and reuse caprolactam, the raw material used to make nylon 6. Honeywell and DSM now manage the largest commercial-scale nylon recycling plant in the world as joint venture partners of Evergreen Nylon Recycling.

The first facility of its kind, the Evergreen Nylon Recycling plant, uses this new process in a true closed-loop depolymerization and purification system that allows whole carpets to be fed into the facility. Expensive mechanical separation/beneficiation is eliminated, and the nylon carpet is converted back to virgin-quality caprolactam. The process is a model of energy efficiency, saving 700,000 barrels of oil and 4.4 trillion Btu annually in comparison to conventional caprolactam production. Although Evergreen is recycling only nylon 6 carpets and post-industrial fiber waste, the technology can be applied to any nylon 6 product, including fibers for commercial and residential carpets, engineered plastics, automotive parts, sporting goods, and films for packaging.

Evergreen will produce approximately 100 million pounds of new caprolactam per year. Honeywell is using the Evergreen caprolactam to produce its Infinity™ Forever Renewable Nylon for all nylon 6 applications.

Mohawk Commercial Carpet is already using Infinity™ to manufacture ten different styles of carpet. Ford is also planning to use Infinity™ in several applications, including a throttle body adapter and an air intake manifold. In the future, Honeywell expects automakers to use Infinity™ for products such as door handles, hood components, and air bags.

DSM will market its share of the recycled caprolactam under the trade name ReCap™, which will be available to the entire merchant caprolactam market. Recap™ will also be used in DSM's downstream nylon polymer products, including carpet spinning chips and DSM Akulon Renew brand of engineering plastic resins.

The technology has won several prestigious awards, including the 1999 Design for Humanity Award for the full-scale commercialization of Infinity™ Forever Renewable Nylon. Evergreen was named "Recycler of the Year" by the Plastic Recycling Division of the Society of Plastics Engineers, and the technology was the runner-up for OIT's 2001 Technology-of-the-Year award.

Evergreen Nylon Recycling Plant in Augusta, GA.

Recovery of Plastics from Auto-Shredder Residue

Argonne National Laboratory has developed and licensed a new process that separates flexible polyurethane foam (PUF) from automobile-shredder residue (ASR), cleaning it to produce high-quality foam that can be used to make new products. The resulting foam meets the performance criteria for new-material carpet padding and for reuse in automotive applications. The technology has been licensed to Salyp Recycling Center of Belgium.

Auto shredders generate about 3 to 5 million tons of automotive shredder residue annually from roughly 10 million junked cars. The cars are shredded to recover metal, leaving about 10,000 tons of PUF, which is landfilled at great expense.

The Argonne process is expected to keep significant amounts of auto scrap out of landfills each year. Potential U.S. energy savings are estimated at around 12 trillion Btu per year. The overall process consists of six basic unit operations: (1) PUF recovery and screening, (2) sizing, (3) washing, (4) rinsing, (5) drying, and (6) baling. The process is fully continuous to minimize materials handling and labor costs.

Following the rinsing step, the process uses a unique dryer that reduces drying time from about 3.5 hours to less than 15 minutes. Widespread use of the Argonne process would create another value-added product for the shredder recycling industry while reducing landfill waste.

Salyp will use the technology in Europe, where the European Union is requiring that waste from scrapped automobiles be reduced by 40% by 2005. In 2000, the technology received the "R&D 100 Award" from *R&D Magazine.*

The Argonne process can be used to recycle a wide variety of auto scrap.

Emerging Technologies

In addition to recently commercialized projects, many projects from the 2001 portfolio have achieved "emerging technology" status. Emerging technologies refer to projects that are expected to become commercially available within the next few years. Emerging technologies from the 2001 Chemical IOF portfolio (many of which are listed in the portfolio of active projects) include the following:

Emerging Chemical IOF Technologies

- Alloys for Ethylene Production
- Catalytic Hydrogenation Retrofit Reactor
- Catalytic Membrane
- Electrodeionization for Product Purification
- Membrane for Olefin Recovery
- Pressure Swing Adsorption (PSA) for Product Recovery
- Production of Succinic Acid from Lignocellulose
- Recovery of Thermoplastics via Froth Flotation
- Sorbents for Gas Separations
- Total Cost Assessment (TCA) Tool

Other Key Emerging OIT Technologies Relevant to the Chemical Industry

- Forced Internal Recirculation Burner
- Gas Leak Detection System
- Low-NOx Process Heating System
- Robotic Tank Inspection System
- Tubular Ultrasound Pipe Inspection System
- Ultrasonic Tank Cleaning
- Waste Heat Process Chiller

2001 Chemical IOF R&D Portfolio

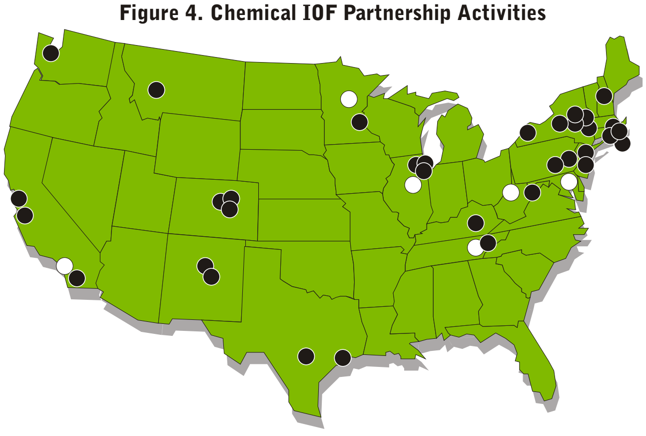
Chemical IOF Projects

In 2001, the Chemical IOF is directly supporting 32 separate R&D projects that pursue priorities outlined in the industry roadmaps. Project topics include: Chemical Synthesis, Bioprocesses and Biotechnology, Materials Technology, Process Science and Engineering Technology, and Computational Technologies.

The Chemical 2001 IOF solicitation process awarded more R&D funding than ever before. This year's solicitation has led to 11 new R&D projects, adding to the team's strong and growing portfolio (see Figure 4.) These projects include:

- Solution Crystallization Modeling Tools
- Distillation Column Modeling Tools
- Enhanced Heat Exchangers for Process Heaters
- Oxidative Olefin Reactor
- High Throughput Catalyst Screening
- Ethylene Process Design Optimization
- Accelerated Characterization of Polymer Properties
- Molecular Simulation for the Chemical Industry
- Membranes for Corrosive Oxidations
- Short-Contact Time Reactors
- Mesoporous Membranes for Olefin Separations

Figure 4. Chemical IOF Partnership Activities



Each of these new R&D projects will last two to three years. DOE will typically provide $250,000 to $750,000 annually, with the industry partners contributing a matching amount. The projects selected in this solicitation stress applied research, show broad applicability within the industry, and meet the criteria of Vision2020.

Small Business Innovative Research (SBIR) Projects

The Chemical IOF R&D portfolio also includes SBIR projects. The SBIR program offers small U.S. businesses an excellent opportunity to partner with the federal government and develop new and energy-efficient technologies. Initial funding begins with the Phase I Award for feasibility testing of a technology that can help advance Chemical IOF goals. Phase II Awards provide additional funding for full-scale research. Through Chemical IOF participation in 2000, SBIR supported to 26 Phase I projects and 8 Phase II projects that pursue chemical industry priorities. In 2001, SBIR supported 15 Phase I projects and 12 Phase II projects.

Other OIT Projects that Benefit the Chemical Industry

In addition to SBIR projects, the Chemical IOF supplements its portfolio by coordinating many projects and activities with other OIT programs. This section highlights just a few of these OIT projects relevant to the Chemical IOF. For a list of additional OIT projects that benefit the Chemical IOF, please see Appendix A.

For fact sheets that provide more detailed information on all these projects, visit the OIT Web site at www.oit.doe.gov or call the OIT Resource Center at (202) 586-2090.

Chemical IOF and SBIR Projects by Topic Area

Chemical IOF Projects	Bioprocesses & Technology	Chemical Synthesis	Computational Technologies	Materials Technologies	Measurement	Process Science and Engineering Technology
Accelerated Characterization of Polymer Properties					X	
Alkane Functionalization Catalysis		X				
Alloys for Ethylene Production*				**X**		
Alloy Selection System				X		
Catalytic Hydrogenation Retrofit Reactor		**X**				
Catalytic Membrane						**X**
Computational Chemistry and Reaction Engineering Workbench			X			
Corrosion Monitoring System				X		
Development of Non-Aqueous Enzymes	X					
Direct Production of Silicones from Sand		X				
Distillation Column Modeling Tools			X			
Electrodeionization for Product Purification						**X**
Enhanced Heat Exchangers for Process Heaters						X
Ethylene Process Design Optimization						X
High Throughput Catalyst Screening		X				
Membrane for Olefin Recovery						**X**
Membranes for Corrosive Oxidations						X
Membranes for p-Xylene Separations						X
Mesoporous Membranes for Olefin Separations						X
Metal Dusting Phenomena				X		
Mixed Solvent Corrosion				X		
Molecular Simulation for Chemical Industry			X			
Multi-Phase Computational Fluid Dynamics			X			
Nanoscale Catalysts		X				
Oxidative Cracking of Hydrocarbons to Ethylene		X				
Oxidative Olefin Reactor		X				
Pressure Swing Adsorption for Product Recovery						**X**
Recovery of Thermoplastics via Froth Flotation						**X**

**IOF Projects classified as Emerging Technologies shown in bold.*

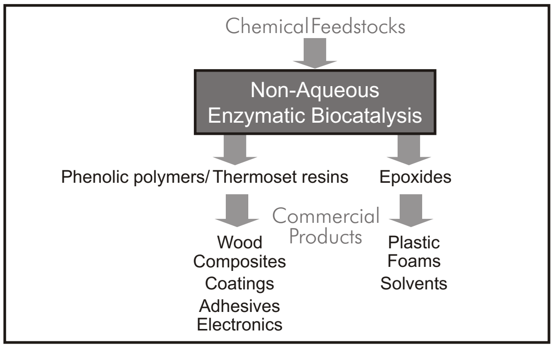
Chemical IOF Projects	Bioprocesses & Technology	Chemical Synthesis	Computational Technologies	Materials Technologies	Measurement	Process Science and Engineering Technology
Selective Oxidation of Aromatic Compounds		X				
Short-Contact Time Reactor		X				
Solution Crystallization Modeling Tools						X
Sorbents for Gas Separations						**X**

Phase I SBIR Projects (awarded in FY 2000)

Phase I SBIR Projects (awarded in FY 2000)	Bioprocesses & Technology	Chemical Synthesis	Computational Technologies	Materials Technologies	Measurement	Process Science and Engineering Technology
Development of Non-Aqueous Enzymes for Chemical Production (1 project)		X				
Membranes for Advanced Industrial Separations (13 projects)						X
Recovery, Recycle, and Reuse of Polymers and Plastics (6 projects)						X
Reactive Separations (6 projects)		X				

Phase II SBIR Projects (awarded in FY 2000)

Phase II SBIR Projects (awarded in FY 2000)	Bioprocesses & Technology	Chemical Synthesis	Computational Technologies	Materials Technologies	Measurement	Process Science and Engineering Technology
Catalyst for CH_4 to CO Conversion		X				
Membrane Module Tubesheet						X
Membrane Reactor for Olefin Production		X				
Nanofiltration of Solvents						X
Phase Transfer Catalysis		X				
Separation of Hydrogen/ Light Hydrocarbon Gas Mixtures						X
Sonic-Assisted Membranes						X
Zeolite Membrane						X



Project Area

Bioprocesses and Biotechnology

Core Portfolio

Development of Non-Aqueous Enzymes

Description

Manufacturers who require polyphenols or propylene oxide (PO) in their production processes may reduce their costs significantly by using biocatalysts (i.e., enzymes) to initiate chemical reactions. This project will develop active and stable biocatalysts for use in organic solvents. If successful, the technology will eliminate the use of formaldehyde, a toxic and carcinogenic chemical, in polyphenol production. Using biocatalysts to produce PO would also prevent the creation of undesirable byproducts and wastes that must be treated.

Benefits
- Energy savings of nearly 70 trillion Btu per year
- Higher yields with less waste
- Increased process efficiency

Partners

Oak Ridge National Laboratory, Massachusetts Institute of Technology, Rensselear Polytechnic Institute, University of California-Berkeley

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Phone: (518) 276-2899
E-mail: dordick@rpi.edu

Amy Manheim
Office of Industrial Technologies

Chemical Synthesis

Core Portfolio

Alkane Functionalization Catalysis

Alkanes are the most abundant and least expensive hydrocarbon feedstock. Alkane functionalization catalysts for the direct conversion of methane to methanol could replace current, energy-intensive methods of methanol synthesis. Project partners are developing a new system to use catalysts that operate in an environmentally-benign media and eliminate the byproduct formation of carbon dioxide, which occurs in the conventional steam reforming process. Considerable opportunities also exist to apply the technology at petroleum drilling sites and extend the system to other alkanes.

Benefits
- Energy savings of nearly 7 trillion Btu per year
- Decreased production of CO_2 by 600,000 tons
- More efficient use of an abundant, inexpensive hydrocarbon feedstock
- Lower operating costs, increased safety, and reduced pollutant emissions

Los Alamos National Laboratory, California Institute of Technology, Akzo Nobel

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Los Alamos National Laboratory
Los Alamos, NM 87545
Phone: (505) 667-9274
E-mail: weg@lanl.gov

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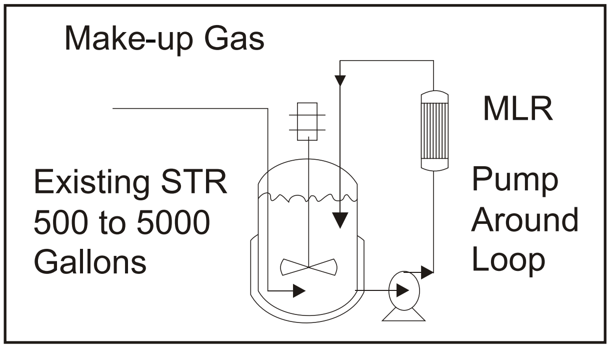
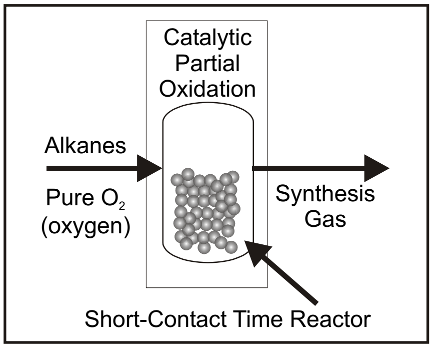
Office of Industrial Technologies



Chemical Synthesis



Chemical Synthesis

Core Portfolio

Catalytic Hydrogenation Retrofit Reactor

This project is developing a fixed bed catalyst system for hydrogenation, a class of chemical reactions performed currently using slurry catalyst systems. A novel catalyst will replace the slurry catalysts that create hazardous wastes and slow productivity in the current process. If successful, the fixed bed catalyst system will be retrofitted to the existing slurry system and will eliminate problems associated with environmental contamination, waste production, productivity, industrial hygiene, and process safety.

Benefits

- Electricity savings of 11% and natural gas savings of 12% per installed unit
- Higher yields
- Decreased operational costs

Air Products and Chemicals, Inc., Johnson Matthey

For additional information please contact:

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Brian Valentine
Office of Industrial Technologies

Core Portfolio

Short-Contact-Time Reactors

Sandia National Laboratories will lead industrial team members in using computational techniques and catalyst characterization to enable the scale-up of a dramatically new process for producing synthesis gas from methane. This synthesis gas process, called catalytic partial oxidation, involves the use of a short-contact time reactor that requires significantly less energy than steam methane reforming. The new reactor utilizes alkanes with pure oxygen to produce synthesis gas.

Benefits

- Reduced capital costs
- High conversion and selectivity
- Elimination of NO_x and CO_2 production
- Reduced fuel consumption

Sandia National Laboratories, Praxair, Inc., Reaction Design, Inc.

For additional information, please contact:

Allen Sault
Sandia National Laboratories
Albuquerque, NM
Phone: (505) 272-7619

Brian Valentine
Office of Industrial Technologies

Process	Waste Generation	Energy Consumption	Cost
Silicon From SiliconDioxide	low	high	moderate
Rochow Direct Process	moderate	moderate	moderate
New Process	low	low	low

Project Area

Chemical Synthesis

Core Portfolio

Direct Production of Silicones from Sand

Description

Project partners are developing a new process for producing silicones that will revolutionize the industry. The chemistry involves creating a new silicon-carbon bonding reaction that will permit numerous silicon-carbon linkages. This process will directly convert silicon dioxide (sand or quartz) into silicone polymers, eliminating the energy-intensive silicon-manufacturing step required in the conventional process. If successful, the technology will reduce many of the wastes generated by present technology and permit the development of new, lower-cost silicone materials.

Benefits

- Up to 47% reduction in energy consumption
- 305,000 tons of coal savings per year
- 95,000 ton decrease in annual solid waste production
- 500,000 ton reduction in CO_2 emissions per year

Partners

General Electric, Molecular Simulation, Inc., OM Group, Inc.

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Amy Manheim
Office of Industrial Technologies

Project Area

Chemical Synthesis

Core Portfolio

High Throughput Catalyst Screening

Description

TDA Research in collaboration with Akzo Nobel is developing a combinatorial catalyst testing apparatus capable of testing an array of catalysts under realistic industrial conditions. The instrument will be an affordable entry point for large and small companies to acquire high throughput catalyst testing capability. Providing such a tool to R&D programs throughout the chemical industry will rapidly accelerate the discovery of new heterogeneous catalysts. The apparatus will be demonstrated initially to screen for new catalysts for the production of ethylene, a highly energy intensive process.

Benefits

- Increased process efficiency
- Decreased need for downstream separations
- Decreased amount of undesired byproducts
- Significant reduction in greenhouse gas emissions

Partners

TDA Research, Akzo Nobel

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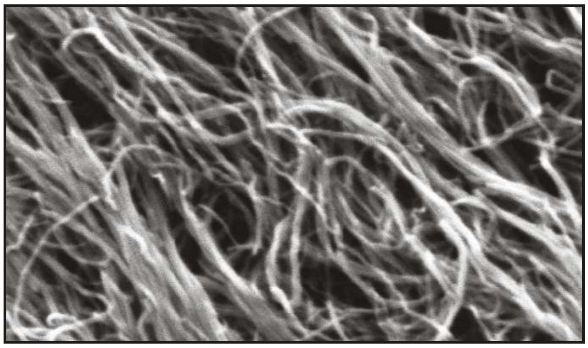
Charles Russomanno
Office of Industrial Technologies



Chemical Synthesis

Core Portfolio

Nanoscale Catalysts

Many chemical reactions require severe, energy-intensive conditions (e.g., high temperatures and pressures, long residence times) or suffer from low product yields because catalysts are not sufficiently selective. This project will develop a new family of catalysts that are more selective, operate at lower temperatures, and increase per pass conversion. The improved performance of these catalysts would reduce energy consumption and associated emissions of pollutants and carbon dioxide from major chemical processes. Specific applications include removal of sulfur from diesel fuel, conversion of n-butane to isobutane (isomerization), and dehydrogenation of ethylbenzene to styrene.

Benefits
- Energy savings of 45 trillion Btu per year
- Reduction in greenhouse gas emissions
- Decreased industrial wastes
- Increased yield and reduced reaction severity

Hyperion Catalysis International, Pacific Northwest National Laboratory, Worcester Polytechnic Institute, Harvard University, University of Utrecht, Washington Group, Inc.

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Hyperion Catalysis
Cambridge, MA
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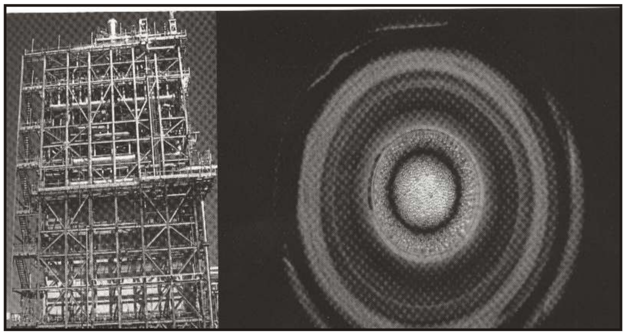

Chemical Synthesis

Core Portfolio

Oxidative Cracking of Hydrocarbons to Ethylene

Ethylene production has been ranked as the most energy-intensive process in the chemical industry, and its demand is growing. A new technology, catalytic autothermal oxydehydrogenation (CAO), could improve the current process by providing high yields of ethylene and other olefins with lower energy requirements and waste generation. Oxidative cracking would no longer require large, inefficient furnaces for heating, nor would it generate coke residue.

Benefits
- Elimination of NO_x via substitution of oxygen for air
- 10-fold reduction in CO_2 generation
- Energy savings of 10 trillion Btu per year

Sandia National Laboratory, Los Alamos National Laboratory, Dow Chemical Company, Reaction Engineering International, University of Minnesota

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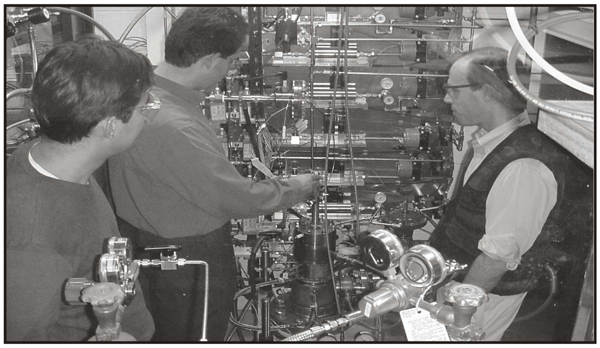

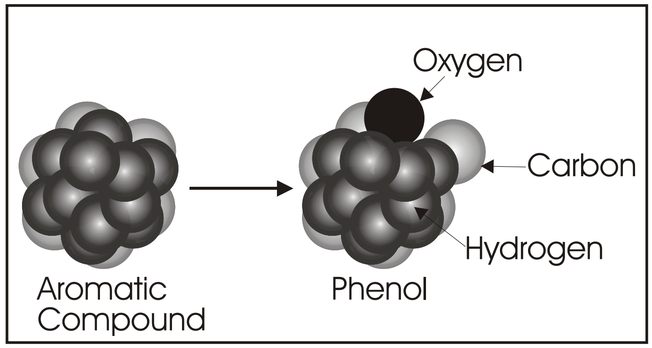

Project Area

Chemical Synthesis | Chemical Synthesis

Chemical Synthesis

Core Portfolio

Oxidative Olefin Reactor

Description

Ethylene is one of the most energy and capital intensive processes in the petrochemicals industry. Project partners are developing a new process for a step-change reduction in capital expenditures and environmental emissions associated with the manufacture of ethylene. This process combines the use of BP's short reaction time catalyst and process knowledge with Praxair's gas mixing technology to provide a novel oxidative dehydrogenation reactor. This process does not require external heat at high temperature as does conventional steam cracking technology. Commercialization will bring about a dramatic reduction in energy consumption and production costs for ethylene manufacture and other similar cracking reactions, including ethylene and propylene production from propane, butane, and naphtha feedstocks.

Benefits
- 20% cost reduction
- Elimination of steam, stack losses, and product compressor
- Reduced reactor capital costs
- Reduced CO_2 emissions

Partners

Praxair, BP, University of Delaware

For additional information, please contact:
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Tarrytown, NY
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E-mail: vasilis_papavassiliou@praxair.com

Dickson Ozokwelu
Office of Industrial Technologies

Chemical Synthesis

Core Portfolio

Selective Oxidation of Aromatic Compounds

Description

Phenol is the second largest commodity produced from benzene. This project involves developing a new one-step process to convert aromatic compounds to phenol. The process would eliminate the need to neutralize acids, separate organic products, or dispose of a potentially unstable intermediate product. The proposed technology would also save energy and reduce byproducts and other hazardous compounds generated by the current three-step process. Significant cost reductions and more effective carbon management would result from the process.

Benefits
- Energy savings of more than 65 trillion Btu per year
- Reduced byproducts and hazardous wastes
- Reduced capital costs
- Minimized production of CO_2
- Utilization of an inexpensive feedstock

Partners

Akzo Nobel Chemicals, Inc., Argonne National Laboratory, Engelhard Corporation, ABB Lummus Global, Northwestern University, Reaction Design, University of Virginia

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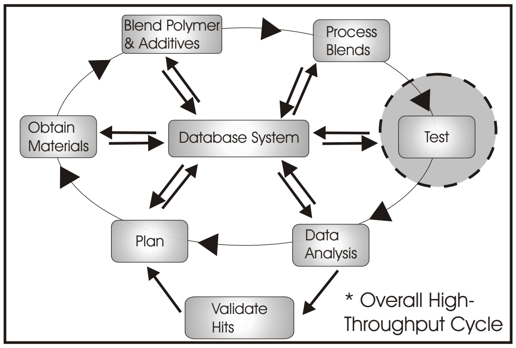
Office of Industrial Technologies



Chemical Measurement

Core Portfolio

Accelerated Characterization of Polymer Properties

Project partners are developing a suite of microanalysis techniques that can rapidly measure a variety of polymer properties of industrial importance. This enabling technology will provide a combinatorial or high-throughput methodology for achieving enhanced polymer performance. Such an approach is expected to revolutionize the polymer and polymer additives industry. Implementation of this technology will result in polymers with enhanced end-use performance, driving plastics into new product lines and markets.

Benefits
- Improved yields of in-specification polyolefin products
- New lightweight application areas for plastic
- At least 10-fold reductions in product development and new product delivery times
- More finely optimized, efficient, and robust plastic products

GE, Cytec Industries, DACA Instruments

For additional information, please contact:
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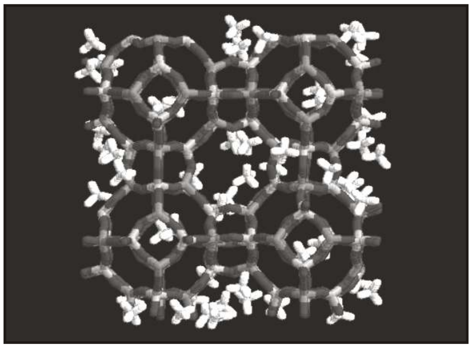
GE Corporate R&D
Niskayuna, NY
Phone: (518) 387-5563

Dickson Ozokwelu
Office of Industrial Technologies



Computational Technologies

Core Portfolio

Molecular Simulation for Chemical Industry

Sandia National Laboratory is leading industrial team members in a project to overcome technology barriers to atomistic-scale simulations for chemical processing. This project addresses two major barriers: poor inter-availability of codes and the unavailibility of validated intermolecular potentials for a wide variety of systems and state conditions. Partners will work together to develop user-friendly codes for steady state equilibrium and fluid phase equilibrium.

Benefits:
- Optimized process with greater efficiency
- Enhances production capacity

Sandia National Laboratories, Air Products and Chemicals, Inc., E.I. DuPont de Nemours & Co., Inc., Ford Motor Company

For additional information, please contact:
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Phone: (505) 284-6355

Brian Valentine
Office of Industrial Technologies

PROJECT AREA

Computational Technologies

Core Portfolio

Computational Chemistry and Reaction Engineering (CCRE) Workbench

DESCRIPTION

This project will develop new software that integrates a suite of computational chemistry tools into a unified package with a graphical, user-friendly interface. The CCRE Workbench will be used in the design and optimization of pyrolysis reactors, boilers and furnaces, and atmospheric reactions. This package will enhance the learning curve required to implement computational tools and increase implementation by plant engineers.

Benefits

- Enhanced process efficiency
- Decreased emissions
- Increased product yield

PARTNERS

Colorado School of Mines, National Renewable Energy Laboratory, Exxon Research and Engineering Company, MC Research and Innovation Center, Gaussian, Inc., Reaction Design, Inc., Adapco Ltd., DuPont, University of Delaware, Wesleyan University, National Institute of Standards and Technology, Lorentzian

For additional information, please contact:
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Office of Industrial Technologies

Computational Technologies

Core Portfolio

Distillation Column Modeling Tools

Project partners are developing advanced computational techniques to model distillation column operation for use in process optimization and the improvement of column packing design. A commercialized software package for use on next generation computers will be made available across the industry to optimize distillation column operations.

Benefits

- Reduced CO_2 emissions
- Significantly increased production capacity
- Improved packing performance and operating conditions
- Reduced energy consumption and waste production

University of Texas–Austin, Oak Ridge National Laboratory, Dow Chemical, Koch-Glitsch, Praxair, Sulzer Chemtech, Fluent, Inc., 3D-1D

For additional information, please contact:
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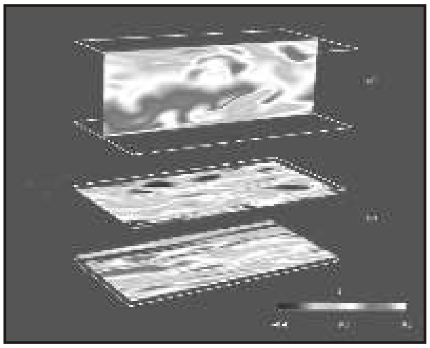

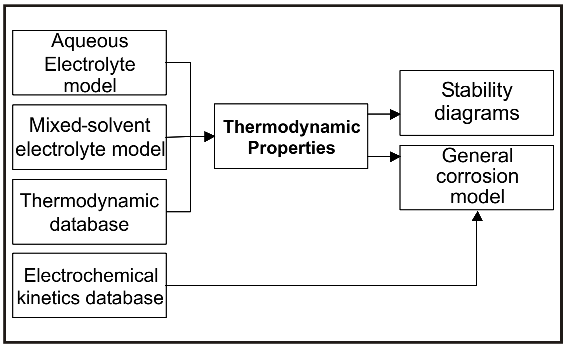

Computational Technologies

Core Portfolio

Multi-Phase Computational Fluid Dynamics (CFD)

The Multi-Phase Fluid Dynamics Research Consortium was established to advance CFD beyond the state-of-the-art achievable by any single business or laboratory. This project partners petrochemical companies, DOE national laboratories, energy equipment manufacturers, and a computer manufacturer. Partners are analyzing dense gas-solid turbulent flows, the industry's highest priority for CFD modeling, to develop software packages for widespread use among chemical and petrochemical companies. This R&D will help industry predict flow properties and improve production under industrial conditions.

Benefits
- Optimized processes with greater energy efficiency
- Increased production capacity

AEA Technology, Chevron, Dow Chemical, Dow Corning, DuPont, Exxon, Fluent, Millennium Inorganic Chemicals, Particulate Solids Rsearch, Inc., Siemens Westinghouse Power Corporation, Argonne National Laboratory, National Energy Technology Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Sandia National Laboratories, Clarkson University, Princeton University, Purdue University, University of Colorado, University of Michigan, Washington University

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Materials Technology

Core Portfolio

Mixed Solvent Corrosion

Since corrosion is difficult to predict in organic or mixed-solvent environments, chemical companies often over-engineer equipment to avoid corrosion failure, costing both money and energy. Project partners are generating computer models to predict corrosion rates in mixed solvent environments and incorporating that data into a commercial software package. Successful completion of this project will prevent future equipment over-design, in addition to reducing energy costs and environmental releases, while increasing productivity.

Benefits
- Energy savings of 33 trillion Btu per year
- Reduction in hazardous disposal of fly ash and particulates by 80%

OLI Systems, Inc., Dow Chemical Company, DuPont Chemical Company, Westvaco, Membrane Technology Institute, Oak Ridge National Laboratory

For additional information, please contact:
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Morris Plains, NJ
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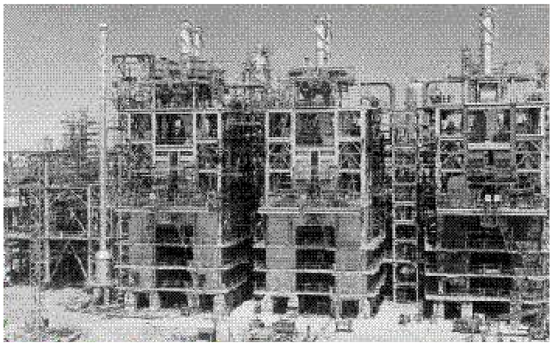
E-mail: mrafal@olisystems.com

Charlie Sorrell
Office of Industrial Technologies

Core Portfolio



ASSET Project Meeting at Oak Ridge National Lab
Oak Ridge, Tennessee, August 17 and 18, 2000

PROJECT AREA

Materials Technology

Core Portfolio

Alloys for Ethylene Production

DESCRIPTION

The decoking necessary to maintain ethylene furnace tubes makes ethylene production one of the most energy-intensive chemical processes. Project partners are developing tubes from iron, nickel aluminide, and advanced metallic alloy materials resistant to the coking and carburization that plague traditional tubes of cast or wrought high-alloy stainless steel. Novel tube fabrication and welding techniques are also being addressed.

Benefits

- Energy savings potential of 20 trillion Btu annually
- Improved equipment life-cycle
- Optimized reaction conditions
- Improved coking resistance

PARTNERS

Exxon Chemical Company, Air Products and Chemicals, Akzo Nobel Chemicals, BP, Duraloy Technologies, Equistar Chemicals, Inco Alloys International, MTI, Nooter Fabricators, Sandvik Steel, Shell Chemical Company, and Oak Ridge National Laboratory

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E-mail: angelinip@ornl.gov

Charles Sorrell
Office of Industrial Technologies

Materials Technology

Core Portfolio

Alloy Selection System

This project aims to improve predictions of corrosion rates for metals and alloys exposed to high-temperature gases. Research will stem from a database and linked thermochemical calculation programs called ASSET. Project partners will enhance the abilities of ASSET to predict corrosion for a much wider range of gases and temperatures. The resulting technology will allow for the selection of more efficient process temperatures and less costly alloys. ASSET optimization will also reduce maintenance costs and carbon dioxide emissions.

Benefits

- Enhanced productivity
- Energy savings of 2%
- Fewer shutdowns due to equipment corrosion
- Reduced CO_2 emissions

Shell Oil Company, Oak Ridge National Laboratory, Humberside Solutions, Ltd., The Royal Military College Of Canada, Ecole Polytechnique de Montreal, Materials Technology Institute, Texaco, Foster Wheeler Development Corporation, Caterpillar, Special Metals Corporation, Haynes International, KEMA (Netherlands), Creusot-Loire

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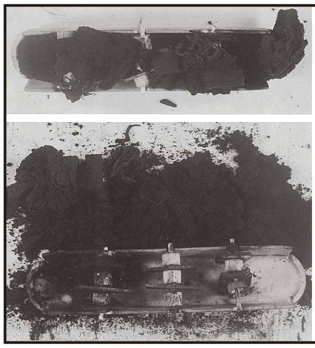
Office of Industrial Technologies



Effects of Metal Dusting

Materials Technology

Core Portfolio

Corrosion Monitoring System (CMS)

Corrosion-related problems cost the U.S. chemical industry millions of dollars annually in energy, waste, and productivity losses. This project seeks to reduce these losses by developing a continuous, on-line CMS. Unlike conventional detection and monitoring systems, this CMS technology will identify existing problems (diagnostics) and predict future failures (prognostics). The system will reduce annual energy usage by decreasing corrosion-related chemical process outages.

Benefits

- Energy savings of 3.54 trillion Btu by 2005
- Increased productivity
- Reduced CO_2 and NO_x emissions
- Significantly reduced downtime

Honeywell, Material Engineering, Oak Ridge National Laboratory, Materials Technology Institute

For additional information, please contact:

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Materials Technology

Core Portfolio

Study of Metal Dusting Phenomenon

Metal dusting is a type of high temperature corrosion that causes unplanned shutdowns. Project partners are studying this phenomenon and developing new alloys and coatings resistant to such corrosion. Project partners also plan to establish a user-friendly database on metal dusting, corrosion, and mechanical properties of materials. Initial applications of the information and materials developed are in hydrogen and synthesis gas production. Other chemical processes, such as methanol production and hydrocarbon and ammonia synthesis, could also benefit from this technology.

Benefits

- Reduced energy consumption
- Greater process reliability
- Lower unit cost of products

Materials Technology Institute, Argonne National Laboratory, Air Products and Chemicals, Inc., DuPont, Exxon Chemical, Honeywell (formerly Alliedsignal), Haynes International, Avesta Sheffield, Sandvik Steel Company, Duraloy Technologies, Special Metals, Allegheny Ludlum Corporation, Krupp VDM

For additional information, please contact:

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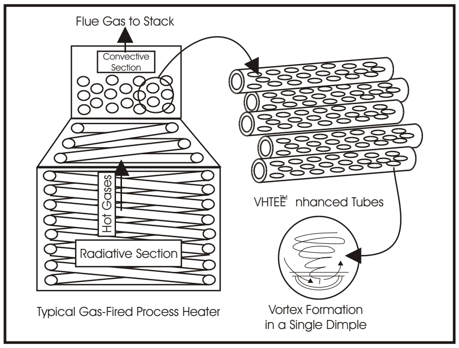
Charles Sorrell
Office of Industrial Technologies

Project Area

Description

Partners



Process Science & Engineering Technology

Core Portfolio

Enhanced Heat Exchangers for Process Heaters

Gas Technology Institute (GTI) and the project partners are working to enhance the overall heat transfer coefficient of the convective section in natural gas-fired (and other-fuels) process heaters using a Vortex Heat Transfer Enhancement (VHTE) approach that can be applied to the many fired process heaters used throughout the chemical industry.

Benefits

- Increased thermal efficiency
- Decreased combustion emission rate

Gas Technology Institute, BP, Exxon Mobil

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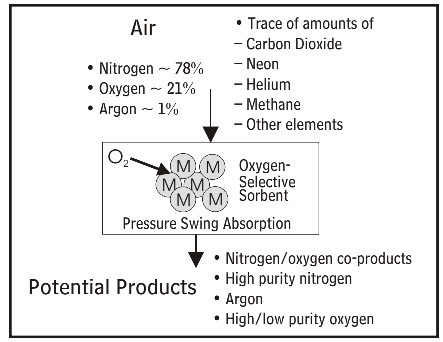

Process Science and Engineering Technology

Core Portfolio

Sorbents for Gas Separation

Project partners are working on a new technology that cost-effectively produces industrial gases such as nitrogen and oxygen. The technology is based on oxygen-selective sorbent materials and pressure swing adsorption (PSA), and will use less energy for gas separation. If successful, the aluminum industry, a major consumer of industrial gases, could use the nitrogen to both prevent oxidation in annealing and other applications and reduce fuel consumption. Inexpensive oxygen would also encourage furnace operators to use oxygen instead of air, further improving energy efficiency and reducing emissions.

Benefits

- Energy savings of 4.2 trillion Btu per year from industrial use of low-cost gas
- Reduced production costs by 25 to 30%
- Energy savings of 2.0 trillion Btu per year in the aluminum industry

Alcoa, Bend Research, Pennsylvania State University, Praxair, Sigma-Aldrich, Inc., University of New Mexico

For more information, please contact:
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Charles Russomanno
Office of Industrial Technologies

Process Science & Engineering Technology

Core Portfolio

Electrodeionization for Product Purification

Electrodeionization is an established technology that combines the features of ion-exchange and electrodialysis to achieve greater efficiency, and eliminate chemical regenerants (acids and bases) and salty waste water streams. Project partners plan to expand electrodeionization, also called "electrochemical ion-exchange," to the chemical industry for economically purifying water, recovering waste, and recycling water. The technology can also handle extremely dilute feed streams of low electrical conductivity, and has potential to handle such challenges as organic foulants, multivalent ions, and an acidic or basic pH.

Benefits

- Energy savings of 5.3 trillion Btu per year
- Reduction in waste water by 61.5 million tons per year
- Reduction in waste salt by 360,000 tons per year

Argonne National Laboratory, NTEC EDSep, Inc., Tate and Lyle

For more information, please contact:
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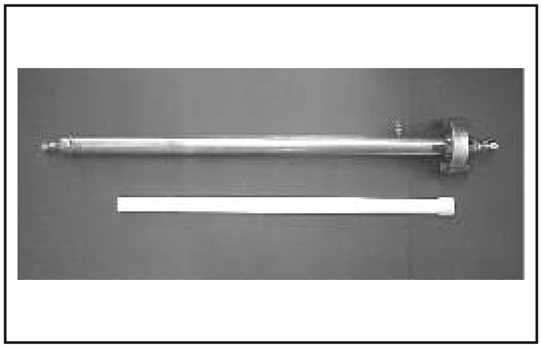

Process Science and Engineering Technology

Core Portfolio

Catalytic Membrane

Ceramic membranes are known for their material stability. Porous ceramic membranes have been widely used commercially in liquid phase separations. This project involves the development of ceramic membranes for gas separations at high temperatures (100 to 600°C). Both the membrane separating layer and a low-cost, high-surface area ceramic membrane support and module are being developed for field implementation. The initial targeted applications are hydrogen production, landfill gas recovery, and CO_2 removal in natural gas processing. Significant energy savings are possible, since cooling prior to gas separations can be eliminated. Furthermore, productivity for certain thermodynamically limited catalytic reactions is improved via high temperature gas separations with the proposed ceramic membranes.

Benefits

- Gas separations energy savings at high temperature
- Improved productivity due to enhanced conversion of chemical reactions
- Simplified chemical production processes

University of Southern California, GC Environmental Co., Media and Process Technology, Inc.

For more information, please contact:
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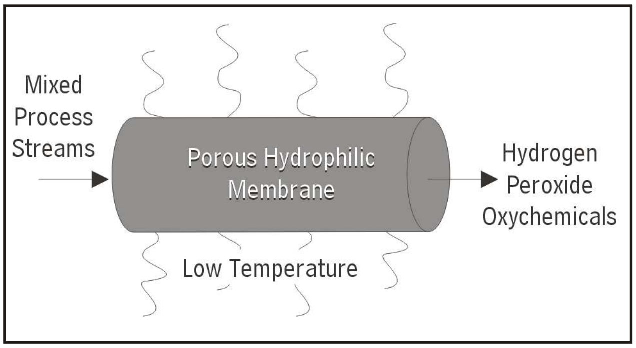

PROJECT AREA

Process Science & Engineering Technology

Core Portfolio

Ethylene Process Design Optimization

DESCRIPTION

Project partners are developing an optimized process configuration for an advanced olefin plant. Since the construction of existing olefin plants significant energy efficient technologies have emerged, many of which have not yet been fully adopted (e.g., advanced separators, furnaces, and cracking tubes). This project will consider the system integration of all modern advancements to olefin plant design, with optimization as the goal.

Benefits
- 15% decrease in energy consumption per pound of product
- 15% lower greenhouse gas emissions per pound of product
- 2% higher process efficiency per pound of product
- 15% reduction in overall cost of production per pound of product

PARTNERS

BP, Aspen Tech

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Charles Russomanno
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Process Science & Engineering Technology

Core Portfolio

Membranes for Corrosive Oxidations

Argonne National Laboratory will lead industrial team members in developing porous hydrophilic membranes highly resistant to oxidative and corrosive conditions. The membranes will then be deployed to recover and purify high-tonnage chemicals such as hydrogen peroxide and other oxychemicals. Hydrogen peroxide is an effective oxidant that produces only water as a byproduct. There is great potential to use hydrogen peroxide in the manufacture of many large-volume commodity petrochemicals via efficient and environmentally friendly processes.

Benefits
- Economical, safe hydrogen peroxide production and utilization
- Avoidance of resultant waste salts
- Reduced steam consumption in distillation
- Significant heat and electrical energy savings

Argonne National Laboratory, UOP LLC, United Technologies, Inc.

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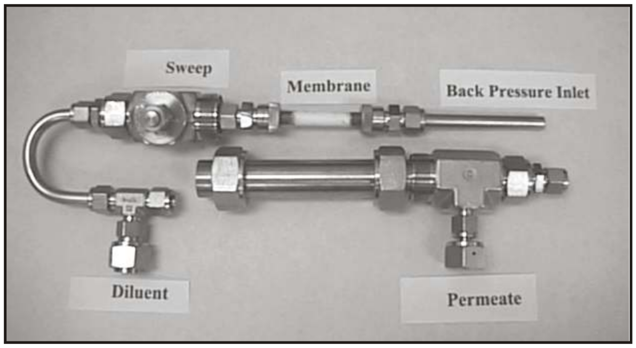

Process Science and Engineering Technology

Core Portfolio

Membranes for p-Xylene Separations

This project aims to help the chemical industry reduce its energy consumption through a new process for use in purified terephthalic acid (PTA) production. Currently, the raw material for PTA is derived from petroleum and requires an energy-intensive process to separate para-Xylene (pX) from a mixture of xylenes. Researchers plan to develop inorganic membranes with improved properties that can separate pX using 75% less energy than the current technology. Project activities include membrane identification, optimization of deposition techniques, and design of a pilot plant for membrane synthesis.

Benefits

- Energy savings of 105 trillion Btu per year
- Reduced capital expenditures in the chemical industry
- Reduced U.S. dependence on imported fossil fuels

Amoco Chemical Company, Sandia National Laboratories, Coors Technical Ceramics

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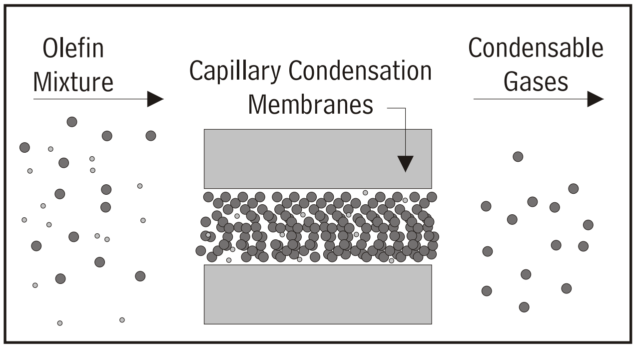

Process Science and Engineering Technology

Core Portfolio

Mesoporous Membranes for Olefin Separations

Los Alamos National Laboratory will lead industrial team members in a project to demonstrate the economic, technical, and commercial potential of a novel membrane separation process for olefin plants. Partners are developing a membrane process to separate olefinic mixtures from light gas byproducts at higher temperatures and lower pressures than currently required in a demethanizer feed chilling system. The end result will be the design of a commercially scalable pilot plant that uses uniquely optimized mesoporous membrane systems to separate olefinic mixtures from light gas byproducts.

Benefits

- Significant reduction in energy consumption
- Decreased CO_2 emissions
- Reduced manufacturing costs
- Cost-effective capacity increases of up to 50%

Los Alamos National Laboratory, BP, MEDAL Air Liquide

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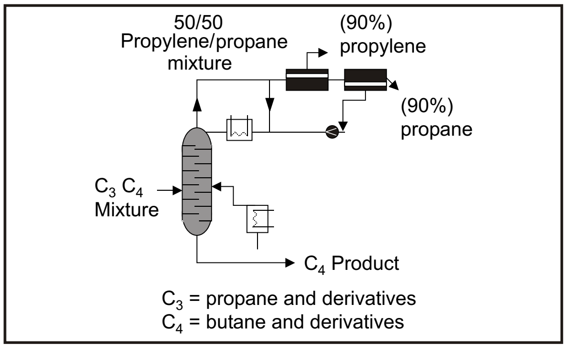

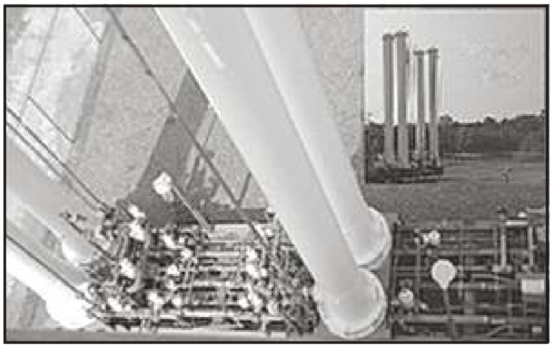

PROJECT AREA

Process Science & Engineering Technology

Core Portfolio

Membrane for Olefin Recovery

DESCRIPTION

This project involves developing polymer membranes to recover olefins (compounds with carbon-carbon double bonds such as ethylene and propylene) from petrochemical byproducts and vent streams. Currently, olefin separation accounts for a major portion of ethylene and propylene production costs. Waste streams containing olefins are then flared or used as a fuel even though the olefin is more valuable as an in-process feedstock. This technology will allow both olefin separation and recycling within the process.

Benefits
- Energy savings of 26.8 trillion Btu per year by 2020 from olefin-containing vent streams in the CPI
- Waste reduction of 1.16 billion pounds per year by 2020
- Recover over 0.68 billion pounds of olefins per year
- Material cost savings—refinery grade olefin feedstock is worth $0.15 per pound whereas olefin used as a fuel is worth $0.04 per pound

PARTNERS

Membrane Technology Research, Inc., BP Chemicals, Phillips Sumika Polypropylene Company

For more information, please contact:
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Charles Russomanno
Office of Industrial Technologies

Process Science and Engineering Technology

Core Portfolio

Pressure Swing Absorption (PSA) for Product Recovery

PSA is an energy-efficient, economical method to recover valuable components from waste streams. This project will identify existing adsorbents, and develop new adsorbents and processes, that allow reliable removal of heavy hydrocarbons currently limiting the performance of PSA systems contained in gas streams. The PSA field unit plans to demonstrate the potential of the new system to use adsorbents for recovering high-value products from polyolefin vent and refinery offgas streams.

Benefits
- Significantly increased hydrocarbons and hydrogen
- Decreased NO_x, CO_2, and VOC emissions
- Reduced operating costs

AirProducts and Chemicals, Inc., University of Kentucky

For more information, please contact:
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Charles Russomanno
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Process Science and Engineering Technology

Core Portfolio

Solution Crystallization Modeling Tools

Project partners are developing tools for engineering design, scale-up, and crystallization process optimization. Crystallization is the most widely used separation and purification process for chemical products that are solids at room temperature and pressure. The new software tools will help design crystallizers for minimum product loss and maximum energy efficiency and product production rate.

Benefits

- Improved heat transfer
- Reduced waste
- Reduced downtime
- Improved filterabilty and mixing efficiency

OLI Systems, Fluent, Inc., Dow Chemical, Eli Lilly, University of Utah, Iowa State University, University of Sheffield, Illinois Institute of Technology, AIChE Design Institute for Physical Property Research

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Charles Russomanno
Office of Industrial Technologies

Process Science and Engineering Technology

Core Portfolio

Recovery of Thermoplastics via Froth Flotation

Froth flotation allows ABS, HIPS, and other plastics of similar densities to be separated. This technology can be applied as a finishing step to conventional separation methods already used for plastics of different densities (e.g., gravity separation). During froth flotation, the surfaces of the plastics are modified by placing them in an aqueous mixture with chemical properties that force HIPS particles to float and separate from sinking ABS particles. Recycling just these two types of plastic could prevent the landfilling of 570 million pounds of auto and appliance scrap annually.

Benefits

- Energy savings of more than 97 trillion Btu per year by 2020
- Waste reduction of more than 800,000 tons annually by 2020
- Decreased greenhouse gas emissions
- Feedstock cost savings of 60% to 80%
- Recovery of 300 million pounds of plastic per year for reuse

American Recycling Partnership, Appliance Recycling Centers of America, Inc., Vehicle Recycling Partnership, Argonne National Laboratory

For more information, please contact:
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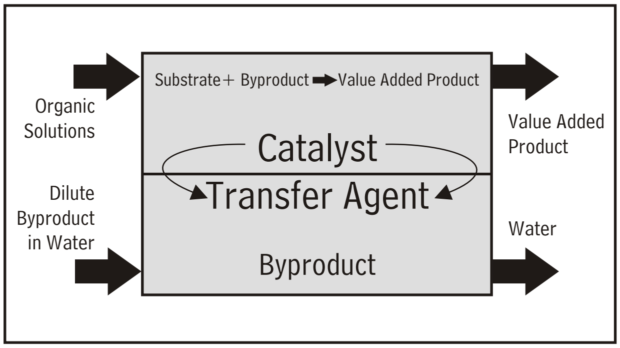

PROJECT AREA

Chemical Synthesis

2000 SBIR Phase I Portfolio

Development of Non-Aqueous Enzymes for Chemical Production

DESCRIPTION

- Molecular Imprinting of Enzymes with Hydrophobic Compounds to Improve Catalytic Activity in Non-aqueous Media; EnzyMed, A Division of Albany Molecular Research Inc., IA

PARTNERS

For more information, please contact:
Charles Russomanno
Office of Industrial Technologies

Chemical Synthesis

2000 SBIR Phase I Portfolio

Reactive Separations

- Novel Membrane Reactor for Fischer-Tropsch Synthesis; CeraMem, MA
- Isobutane Isomerization Membrane Reactor; Membrane Technology and Research, Inc., CA
- High-Octane Fuel Stock via Reactive Separation; Epsilon, Inc., NJ
- Low Energy Separation of Azeotropes by Gel Absorption; Foster Miller, Inc., MA
- Nanopore Silica Reactive Adsorbent; Industrial Science and Technology Network, Inc., PA
- A Membrane Reactor for High Density Hydrogen Production at 100% Purity; REB Research and Consulting, MI

For more information, please contact:
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Process Science and Engineering

2000 SBIR Phase I Portfolio

Membranes for Advanced Industrial Separations

- High-Selectivity Membranes for Olefin/Paraffin Separations; Bend Research, Inc., OR
- Corrosion Resistant Honeycomb Ceramics for Economical Membrane Separation of Industrial Wastewater; Applied Ceramics, Inc., GA
- Affinity Ceramic Membranes with CO_2 Transport Channel; Media and Process Technology, Inc., PA
- Membranes For Reverse Organic Air Separations; Compact Membrane Systems, Inc., DE
- Low Cost Silicon Carbide Ceramic Membranes; Custom Materials, Inc., MD
- Hydrogen Recovery Process Using New Membrane Materials; Membrane Technology and Research, Inc., CA
- Ceramic Appliques For the Production of Supported Thin Film CMRs; Eltron, CO
- Photocatalytic Membranes for Producing Ultrapure Water; Technology Assessment and Transfer, Inc., TTM, MD
- Ceramic Membrane Process For Upgrading Vacuum Residual Oil; CeraMem Corporation, MA
- A Novel Inorganic Surface Diffusion Membrane For Hydrogen Separations; TDA Research, Inc., CO
- Low-Cost, High-Purity Ionic Transport Ceramic Oxygen Generator; Energy Research Company, NY
- Mercury-Binding Membranes For Flue Gas Cleanup; TPL, Inc., NM
- Harsh Fluorochemical Separations; Compact Membrane Systems, Inc., DE

For more information, please contact:
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Process Science and Engineering

2000 SBIR Phase I Portfolio

Recovery, Recycle, and Reuse of Polymers and Plastics

- Phenol/Neutrals Production from Recycling Carbon/Epoxy Composites; Adherent Technologies Inc., NM
- Mechanical Paint Removal Technology for Commercial Recycling of Engineering Thermoplastics; Regrind Services, LLC, MI
- Low Temperature Composite Recycling Process; Adherent Technologies, Inc., NM
- Development of Data Processing Scheme for Plastic Identification Instruments; Physical Sciences Inc., MA
- Separation and Recovery of Thermoplastics for Re_Use via Froth Flotation from Nylon Production Waste Streams; SDR Plastics, Inc., WV
- The Use of Recycled Plastics as Alternative Soil Amendments in the Culture of Plants, AgBio Development Inc., CO

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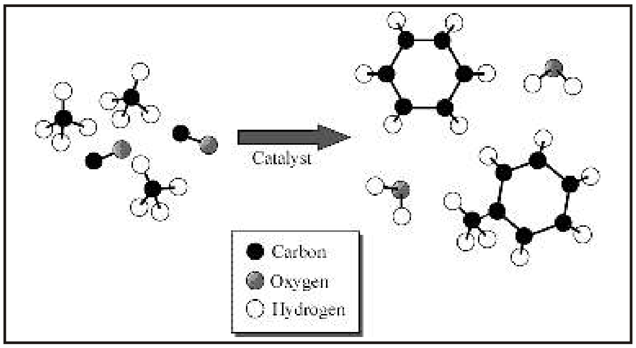

Project Area

Chemical Synthesis

2000 SBIR Phase II Portfolio

Catalyst for CH_4 to CO Conversion

Description

High cost and inefficient processes have limited the feasibility of large-scale production of liquid chemicals from the U.S. domestic coal and natural gas supply. Project partners are addressing these issues by developing a catalyst that directly converts methane to aromatics (benzene, toluene, xylene, and napthalene) and light olefins. Successful completion of this project will provide a significant increase in the utilization of domestic and remote natural gas reserves because the technology directly converts natural gas to higher molecular weight products of substantially higher market value.

Benefits

- More efficient use of domestic and remote gas sources
- Decreased oil import expenditures

Partners

CeraMem Corporation, UOP LLC, Zeolyst International, Dynamism Technical Services, Inc.

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Charles Russomanno
Office of Industrial Technologies

Chemical Synthesis

2000 SBIR Phase II Portfolio

Membrane Reactor for the Production of Olefins

This membrane reactor will significantly reduce the production costs of olefin, a key feedstock in the chemical industry. The technology increases equilibrium conversion and reduces the size of the production separation step. Dehydrogenation of propane is the most commercially important application that would arise from this technology. In Phase I, the membrane reactor was devised and modeled on a computer process simulator. In Phase II, Membrane Technology and Research, Inc. (MTR) is scaling up to large membrane modules and conducting tests first in laboratories and then at field sites.

Benefits

- Reduced CO_2 emissions
- Increased productivity

Membrane Technology and Research, Inc., Georgia Institute of Technology

For more information, please contact:
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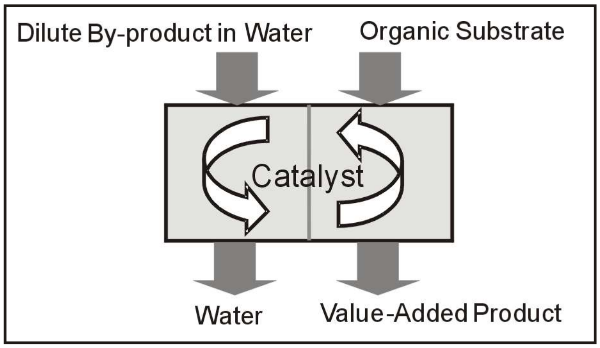

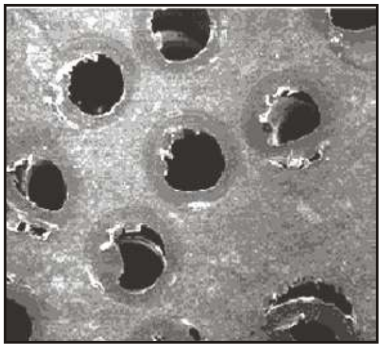

Chemical Synthesis

2000 SBIR Phase II Portfolio

Phase-Transfer Catalysis (PTC)

PTC is a method for converting dilute byproduct streams into value added products rather than greenhouse gases or other wastes. PTC can be applied to a wide variety of byproduct streams in the chemical processing industry. PTC can be used in the production of adhesives, polymers, explosives, petroleum, flavors, and fragrances. Phase I validated project methodology by extracting phenol and phenol derivatives from hazardous waste and byproduct streams. Phase II is exploring other applications for PTC and developing reaction engineering for the systems.

Benefits

- Reduced CO_2 emissions by 78,000 tons per year
- Reduced waste treatment costs
- Reduced hazardous waste
- Enhanced byproduct reactivity

PTC Value Recovery, Hercules Inc., PTC Organics, Widner University, CINC Inc., Iowa State University, New Jersey Commission on Science

For more information, please contact:
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Office of Industrial Technologies

Chemical Synthesis

2000 SBIR Phase II Portfolio

Membrane Module Tubesheet

Many process streams chemically attack materials used to seal tubes, or are at temperatures above the working limits of epoxy tubesheets. Making epoxy tubesheets with improved mechanical properties, chemical and thermal stability, and resistance to organic solvents, the range of membrane applications will increase dramatically. Improved tubesheets will allow fiber membrane separations to replace distillation in chemical refineries.

Benefits

- Reduced energy consumption by 200 trillion Btu per year
- Improved hardness
- Improved module barrier properties
- Greater adhesive bond strengths

TDA Research, Inc., Air Products Perma Division

For more information, please contact:
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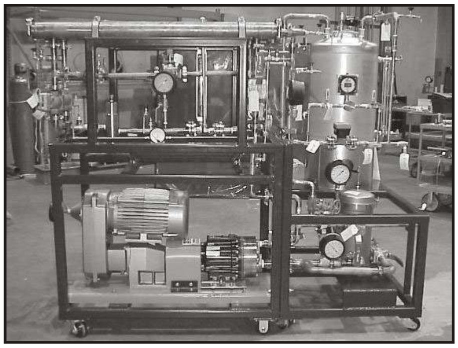

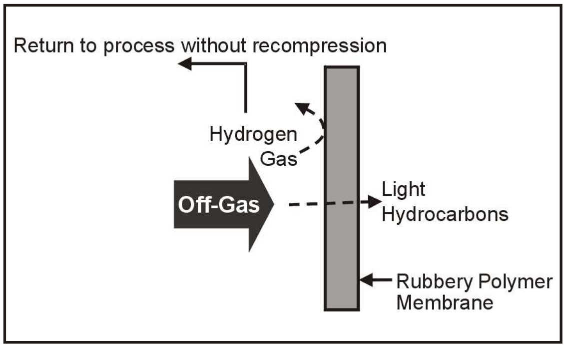

PROJECT AREA

Chemical Synthesis

2000 SBIR Phase II Portfolio

Nanofiltration of Solvents

DESCRIPTION

Many distillation processes involve separation of small molecules from large ones, such as solvents from oils. This project involves developing solvent-resistant selective membranes that can perform these separations and reduce the size of the distillation recovery process. These composite nanofiltration membranes are comprised of a thin mesoporous selective layer coated onto microporous support.

Benefits
- High fluxes
- Resistance to organic solvents
- Operational cost savings

PARTNERS

Membrane Technology and Research, Inc.

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Charles Russomanno
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Process Science and Engineering

2000 SBIR Phase II Portfolio

Separation of Hydrogen/Light Hydrocarbon Gas Mixtures

Hydrogen/light hydrocarbon gas mixtures, produced throughout the refinery and petrochemical industries, are generally used as fuels even though they are three times as valuable when separated. The goal of this project is to develop an economical process for this separation. Phase II is developing membranes for pilot plant tests. The most promising streams for early adaption of this technology are petrochmical hydrogenation vent streams, pressure swing adsorption tail gas, and refinery hydrotreater-hydrocracker purge gas.

Benefits
- Reduced waste from process gas streams
- Decreased production costs

Membrane Technology and Research, Inc., Equilon Enterprises, LLC

For more information, please contact:
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Charles Russomanno
Office of Industrial Technologies

Process Science and Engineering

2000 SBIR Phase II Portfolio

Zeolite Membrane

Zeolite membranes provide several key advantages over other membranes, including high temperature stability, inertness to organic media, and remarkable separation selectivities. The technology would significantly reduce energy use and costs in the petroleum refining, petrochemical, chemical, high-purity gas, and environmental industries. Applications for these industries include light gas separations, close-boiling hydrocarbon separations, dehydration of organic fluids, removal of organics from aqueous streams, and hydrogen recovery.

Benefits
- Continuous operation at high temperatures
- Low operation cost

CeraMem Corporation, University of Colorado, Medal LP

For more information, please contact:
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E-mail: higgins@ceramem.com

Charles Russomanno
Office of Industrial Technologies

2001 SBIR Phase I Portfolio

Reactive Separations

PBO Films as Templates for Production of High Efficiency Nanoporous Composite Membranes
— Foster-Miller, Inc, MA

Reactive Separation via a Hydrothermally Stable Hydrogen Selective Membrane
— Media and Process Technology, Inc., PA

A Novel Taylor Vortex Extractive-Reaction Process for Reducing Organic Wastes Dissolved in Aqueous Streams
— PTC Value Recovery, NJ

A Low-Cost System for the Conversion of HCl to Cl_2
— TDA Research, Inc., CO

Novel Membrane Reactor for the Desulfurization of Transportation Fuels
— Trans Ionics Corporation, TX

Membranes for Advanced Industrial Separations Technology

Low-Cost Ceramic Modules Incorporating Palladium-Based Membranes for Dehydrogenation Reactions
— CeraMem Corporation, MA

Low Emission Diesel Engines
— Compact Membrane, DE

Selective Adsorption Membranes for the Production of Enriched Air
— ITN Energy Systems, Inc., CO

Treatment of Produced Water with Fouling-Resistant Nanofiltration Membranes
— Membrane Technology and Research, Inc., CA

An Acoustically Enhanced Pervaporation Bioreactor (APB)
— Montec Research, MT

Novel Thin-Film Ceria Membrane Materials for Small-Scale Oxygen Generation Systems
— NexTech Materials, Ltd., OH

Recovery, Recycle, and Reuse of Energy Intensive Materials

Recycling of Polystyrene Packaging from the Food Service Industry
— Adherent Technologies, Inc., NM

Recycling of Coated Plastics Used in Automotive, IT and Commercial Applications
— METSS Corporation, OH

Development of a Universal Plastic Resin Composition Sensor for Whole Parts and Reground Mixtures
— Spectracode, Inc., IN

2001 SBIR Phase II Portfolio

Reactive Separations

Novel Membrane Reactor for Fischer-Tropsch Synthesis
— CeraMem Corporation, MA

High-Octane Fuel Stocks via Reactive Distillation
— Epsilon Technologies, NJ

Isobutane Isomerization Membrane Reactor
— Membrane Technology and Research, Inc., CA

Membranes For Advanced Industrial Separation Technology

Ceramic Membrane Process for Upgrading Vacuum Residual Oil
— CeraMem Corporation, MA

Harsh Fluorochemical Separation
— Compact Membrane Systems, Inc., DE

Membranes for Reverse Organic-Air Separations
— Compact Membrane Systems, Inc., DE

Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors
— Eltron Research, Inc., CO

Affinity Ceramic Membranes with Carbon Dioxide Transport Channel
— Media and Process Technology, Inc., PA

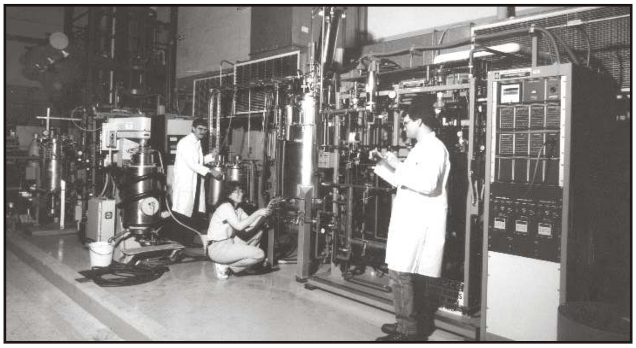
Hydrogen Recovery Process Using New Membrane Materials
— Membrane Technology and Research, Inc., CA

Photocatalytic Membranes for Producing Ultrapure Water
— Techology Assessment & Transfer, Inc., MD

Recovery, Recycle, and Reuse of Polymers and Plastics

Low-Temperature Composite Recycling Process
— Adherent Technologies, Inc., NM

Development of Data Processing Scheme for Plastic Identification Instruments
— Physical Sciences, Inc., MA



Project Area

Bioprocesses and Biotechnology

Other IOF Portfolio

Production of Succinic Acid from Lignocellulose

Description

Although succinic acid is not currently a commodity chemical, it has the potential to compete with chemicals produced from petroleum-based feedstocks. Partners will focus on developing a novel fermentation process to produce succinic acid from a newly engineered bacteria (AFP111). Genetic engineering will ensure that the bacteria is capable of converting different types of sugars efficiently. The process would significantly reduce the use of petroleum resources and consume carbon dioxide. The competitively priced succinic acid produced from AFP111 could be used directly for or as a precursor to many industrial chemicals required for the manufacture of paints, plastics, and other products.

Benefits

- Energy savings of 9.8 trillion Btu per year
- 252,000 tons of waste saved per year
- CO_2 consumed during the fermentation process

Partners

Applied Carbo Chemicals, Argonne National Laboratory, Arkenol, Oak Ridge National Laboratory

For additional information, please contact:
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Oak Ridge, TN 37831
Phone: (865) 576-8522
E-mail: davidson@ornl.gov

Amy Manheim
Office Of Industrial Technologies

Combustion

Other IOF Portfolio

Integrated Process Heater System

Project partners are developing and demonstrating the technology base for a new generation of process heaters both highly efficient and extremely low in emissions. This innovative system incorporates four advanced technologies: an ultra-low emissions smart burner, a fired heater optimized for burners, an on-line tube temperature and burner control system, and an adaptive, predictive emissions monitoring system. The technology will have applications for a broad range of refining and chemical processes. Advanced system components will be developed for use in both new and retrofit applications.

A.D. Little, Inc., ExxonMobil Research and Engineering Company, Callidus Technologies, Inc., GTI

For additional information please contact:
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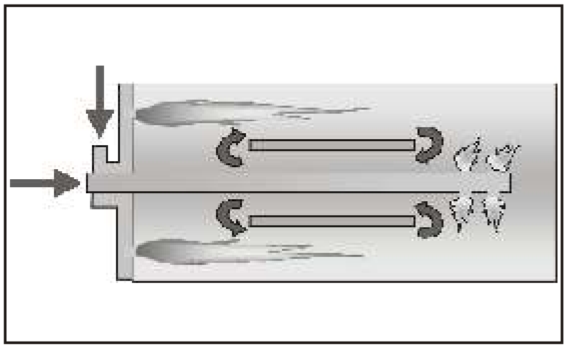
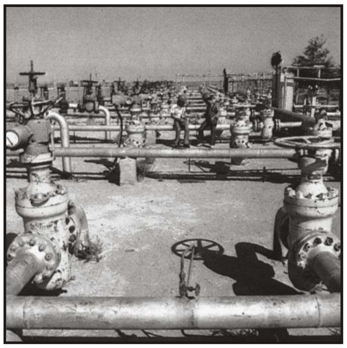
A.D. Little, Inc.
Cambridge, MA
Phone: (617) 498-5844
E-mail: loftus.p@adlittle.com

Robert Gemmer
Office of Industrial Technologies





Combustion

Materials

Other IOF Portfolio

Low-NO_x Forced Internal Recirculation (FIR) Burner

The FIR Burner combines several techniques to dramatically reduce NO_x and carbon monoxide emissions from natural gas combustion without sacrificing boiler efficiency. It uses staged combustion with forced internal recirculation of products of partial combustion. The FIR burner is applicable to a wide range of watertube boilers used in the paper, chemicals, petroleum refining, steel, and food industries.

Benefits

- NO_x emissions below 9ppm
- Increased system efficiency, with operation at less than 10% excess air
- Reduced developmental, operating, maintenance, and capital costs

Institute of Gas Technology and its Sustaining Membership Program, Detroit Stoker Company, Gas Institute of Ukranian National Academy of Sciences, University of Illinois at Chicago, Gas Research Institute

For more information, please contact:
Robert Gemmer
Office of Industrial Technologies

Other IOF Portfolio

Global On-Stream Inspection for Mechanical Integrity

This project will develop on-line inspection and diagnostic technologies to detect, locate, and characterize piping and vessel cracking. The proposed inspection system would assure mechanical integrity, detect cracking before equipment failure occurs, and reduce the number of plant inspections required. Successful implementation of this technology would result in fewer plant shutdowns and therefore increased efficiency and productivity.

Benefits:

- Increased productivity
- Reduced refinery downtime
- Reduced potential of releases to the ground, water, and air
- Extended equipment lifetime

Lawrence Berkeley Laboratory, Ohio State University, Industrial Advisory team

For additional information please contact:
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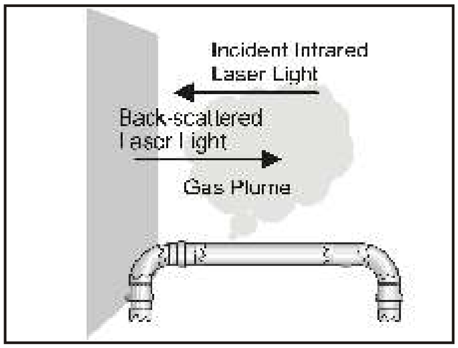
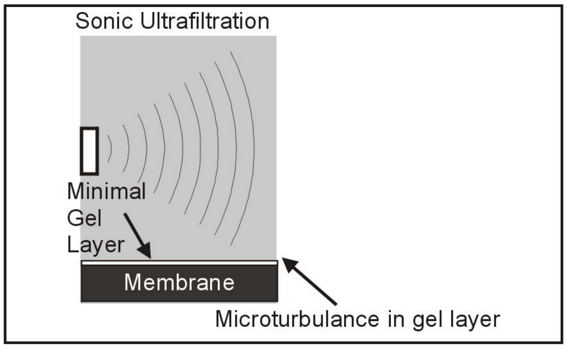
Office of Industrial Technologies





PROJECT AREA

Measurement

Other IOF Portfolio

Gas Imaging Leak Detector

DESCRIPTION

Project partners are developing a gas imaging system for leak detection that will ultimately be person-portable. Gas imaging provides a streamlined alternative to current leak detection, which is often inefficient. The gas imaging system will reduce resource loss and increase energy savings by allowing a refinery to perform more frequent inspections and repair leaks more rapidly.

Benefits:

- Accelerated and simplified leak detection
- Efficient alternative to EPA method 21 leak measurement protocol
- More frequent monitoring surveys

PARTNERS

American Petroleum Institute, Laser Imaging Systems, Sandia National Laboratories, U.S. DOE Office of Oil and Gas Technology, U.S. Environmental Protection Agency

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Gideon Varga
Office of Industrial Technologies

Process Science and Engineering

Other IOF Portfolio

Sonic-Assisted Membranes

Advanced means to filter products of many chemical processes can improve membrane separator performance and increase efficiency. The proposed technology uses high-intensity, low-frequency acoustic energy to improve filtering methods. Sonic-assisted ultrafiltration can be used to remove and prevent build-up of foulants, and to increase flux. Applications include traditional fermentation processes, food processing, chemical manufacturing, municipal water treatment, and waste treatment.

Benefits

- Reduced maintenance costs
- Increased number of biological applications for membranes

Montec Research, Dow Chemical Company

For more information, please contact:
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Charles Russomanno
Office of Industrial Technologies

Process Science and Engineering

Other IOF Portfolio

Robotics Tank Inspection System

Project partners have used NICE^3 funding to demonstrate Maverick, a robotics inspection system designed to eliminate the expense of draining, cleaning, and ventilating tanks prior to inspection. The system inspects the bottoms of aboveground storage tanks containing petroleum and other petrochemical products while they remain in service. The system can reduce inspection costs by $50,000 to $500,000 per tank by eliminating draining, cleaning, and downtime.

Benefits
- Estimated energy savings near 12 trillion by 2010
- CO_2 emission reductions exceeding 8,000 tons per year
- Billions of dollars of savings for the petroleum and chemical industries

Solex Environmental Systems, Inc., Texas Natural Resource Conservation Commission

For additional information please contact:
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Houston, TX
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E-mail: drh@solexrobotics.com

Lisa Barnett
Office of Industrial Technologies

Process Science and Engineering

Other IOF Portfolio

Ultrasonic Tank Cleaning

This technology uses ultrasonic or high-frequency sound waves to generate bubbles in fluid-filled tanks, cleaning inner surfaces without solvents, emissions, or manual labor. The bubbles are small enough to penetrate even microscopic crevices, so the cleaning process is superior to conventional methods. The faster cleaning cycle provides substantial energy savings. Ultrasonic tank cleaning can be used to clean residue from tanks used in chemical and pharmaceutical processing.

Benefits
- Elimination of VOC-emitting cleaning solvents and VOC emissions from the incineration of spent solvent
- Conservation of petroleum feedstocks
- Energy savings of 225 million Btu per year for a 200-gallon tank system

DuPont-Merck Pharmaceutical Company, New Jersey Department of Environmental Protection, TELESONIC Ultrasonics

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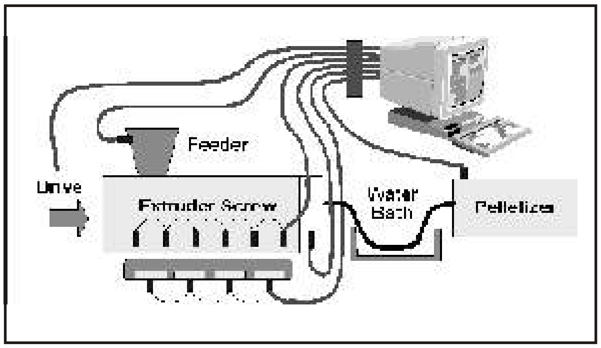

PROJECT AREA

Process Science and Engineering

Other IOF Portfolio

Intelligent Extruder

DESCRIPTION

The intelligent extruder system will use advanced diagnostic and control tools to reduce product variability and increase first-pass yield, while reducing energy use and waste generation, in the compounding of polymer resin. The improved control of extruder operation is becoming critically important as the molding industry moves toward narrowing acceptable quality limits on extruded polymer resins. Although this sensors and controls technology targets the extruded and molded plastics industry for primary use, the core modeling, analysis, and feature extraction tools developed under this project would be readily transportable across implementation platforms and beyond the extruded product industries.

Benefits
- Two percent increase in first-pass yield
- Estimated $780 million annual savings
- Energy savings of 0.02 quads per year
- Waste reduction of 80 tons of volatiles and 820,000 tons of solids per year

PARTNERS

General Electric, General Electric Plastics, Krupp Werner-Pfleiderer Corporation

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E-mail: timothy.cribbs@indsys.ge.com

Gideon Varga
Office of Industrial Technologies

Process Science and Engineering

Other IOF Portfolio

Waste Heat-Driven Process Chiller

When the amount of waste gas exceeds the requirements of refinery furnaces and boilers, the excess (including a small amount of propane) is flared. If that propane can be recovered, the refinery can sell it in the form of liquefied propane gas or gasoline. By chilling the waste gas using a waste-heat-powered absorption refrigeration unit (ARU), about half the propane can be condensed. The ARU is directly integrated into the refinery process and uses enhanced, highly compact heat and mass exchangers. This technology is widely applicable to many industries, not just refinieries, and can be used in mainstream industrial refrigeration applications.

Benefits:
- Recovers 2.1 million gallons of gasoline and liquefied petroleum gas per year
- Decreases annual CO_2 emissions by 10,000 tons per year
- Realizes increased profit of $900,000
- Payback of less than two years

Utlramar Diamond Shamrock, Energy Concepts, Planetec

For additional information please contact:
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Annapolis, MD
Energy Concepts
Phone: (410) 266-6521
Email: enerconcep@aol.com

David Salem
Office of Industrial Technologies

Process Science and Engineering

Other IOF Portfolio

Pipe Inspection System

Project partners have developed a technology to detect and classify defects and imperfections in tubular goods using electromagnetic acoustic transducers (EMAT) technology. This innovative approach uses ultrasonic waves, launched around the tube, to detect manufactured or service-induced defects such as cracks, pitting, and general wall loss. Applications for chemical companies that depend on pipes to move product are possible.

Benefits

- Non-destructive materials analysis
- On-line inspection capability
- Lower maintenance costs

For additional information please contact:

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Tubular Ultrasound LLP
The Woodlands, TX
Phone: (713) 426-1072
david@tubularultrasound.com

Lisa Barnett
Office of Industrial Technologies

Other IOF Portfolio

Appendix A: Other OIT Projects

OIT funds many projects benefitting the chemical industry that are not managed by the Chemical IOF. The following is a list of OIT projects funded by other OIT programs. When available, the location of fact sheets for these projects has been provided.

Projects that Relate Directly to the Chemical Industry

Bioprocesses and Biotechnology

Advanced Biocatalytic Processing of
Heterogeneous Lignocellulosic Feedstocks to a
Platform Chemical Intermediate
Mark Paster
Phone: (202) 586-2821
E-mail: mark.paster@ee.doe.gov

Catalytic Upgrading of Glucose
Mark Paster
Phone: (202) 586-2821
E-mail: mark.paster@ee.doe.gov
Http://www.oit.doe.gov/agriculture/fs_glucose.shtml

Chemical Synthesis

High Temperature Facilitated Membranes
Charles Sorrell
Phone: (202) 586-1514
E-mail: charles.sorrell@ee.doe.gov

Improved Alkylation Contactor
Lisa Barnett
Phone: (202) 586-2212
E-mail: lisa.barnett@ee.doe.gov
Http://www.oit.doe.gov/inventions/pdfs/projects
/iofs/factsheets/vhp.pdf

Materials

Carbon Membranes for Light Gas
Separations
Mike Soboroff
Phone: (202) 586-4936
E-mail: mike.soboroff@ee.doe.gov

Materials for Electrochemical Reactors
Charles Sorrell
Phone: (202) 586-1514
E-mail: charles.sorrell@ee.doe.gov
http://www.oit.doe.gov/factsheets
/chemicals/pdfs/ecreactors.pdf

Oil Refinery Pipe Hangers
Mike Soboroff
Phone: (202) 586-4936
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http://www.oit.doe.gov/factsheets/cfcc/pdfs/pipe_hangers.pdf

Remote Automatic Material On-Line Sensor
Gideon Varga
Phone: (202) 586-0082
E-mail: gideon.varga@ee.doe.gov
http://www.oit.doe.gov/factsheets/sens_cont/pdf/online.pdf

Selective Inorganic Thin Films
Mike Soboroff
Phone: (202) 586-4936
E-mail:mike.soboroff@ee.doe.gov
http://www.oit.doe.gov/factsheets/pdfs/membrane.pdf

Process Science and Engineering Technology

Conducting Polymers
Charles Sorrell
Phone: (202) 586-1514
E-mail: charles.sorrell@ee.doe.gov

Energy Saving Separations Technologies
Amy Manheim
Phone: (202) 586-1507
E-mail: amy.manheim@ee.doe.gov
http://www.oit.doe.gov/factsheets
/petroleum/pdf/separations.pdf

Environmental Assessment of Low
Temperature Plasma Technologies for Treating VOC's from Pulp
Mills and Wood Products Plants
Valri Robinson
Phone: (202) 586-0937
E-mail: valri.robinson@ee.doe.gov
http://www.oit.doe.gov/forest/experimental_assessment.shtml

Distillation Column Flooding Predictor
Rolf Butters
Phone: (202) 586-0984
E-mail: rolf.butters@ee.doe.gov

Separation of Aromatic Isomers
Lisa Barnett
Phone: (202) 586-2212
E-mail: lisa.barnett@ee.doe.gov

Measurement Technologies

Pulsed Laser Imager for Detecting Emissions of Hydrocarbons and VOCs
Lisa Barnett
Phone: (202) 586-2212
E-mail: lisa.barnett@ee.doe.gov

Micro-GC Controller
Robert Gemmer
Phone: (202) 586-5885
E-mail: robert gemmer@ee.doe.gov
http://www.oit.doe.gov/factsheets
/petroleum/pdf/microgcontroller.pdf

Solid State Chemical Sensors for
Monitoring Hydrogen in IOF Process Streams
Gideon Varga
Phone: (202) 586-0082
E-mail: gideon.varga@ee.doe.gov
http://www.oit.doe.gov/factsheets/sens_cont/pdf/hydrogen.pdf

Projects that Are Relevant to the Chemical Industry

Aluminum

Aluminum Salt Cake
Simon Friedrich
Phone: (202) 586-6759
E-mail: simon.friedrich@ee.doe.gov
http://www.oit.doe.gov/aluminum/alumfacts/saltcake12.shtml

High-Heat Transfer Low-NOx Natural Gas Combustion System
Elliott Levine
Phone: (202) 586-1476
E-mail: elliott.levine@ee.doe.gov
http://www.oit.doe.gov/aluminum/pdfs/lownox4.pdf

Combustion

Development of An Innovative Energy
Efficient High Temperature Natural Gas Fired Furnace
Lisa Barnett
Phone: (202) 586-2212
E-mail: lisa.barnett@ee.doe.gov
http://www.oit.doe.gov/factsheets
/combustion/pdfs/gasfurnace.pdf

Super Boiler: Packed Media/Transport
Membrane Boiler Development and Demonstration
Robert Gemmer
Phone: (202) 586-5885
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Forest Products

Bubble Size Control to Improve Oxygen-Based Bleaching
Valri Robinson
Phone: (202) 586-0937
E-mail: valri.robinson@ee.doe.gov
http://www.oit.doe.gov/forest/bubblesize.shtml

Guided Acoustic Wave Monitoring of
Corrosion and Erosion in Recovery Boiler Tubing
Gideon Varga
Phone: (202) 586-0082
E-mail: gideon.varga@ee.doe.gov
http://www.oit.doe.gov/forest/guidedacoust.shtml

Stability and Regenerability of Catalysts for
the Destruction of Tars from Biomass and Black Liquor
Charles Russomanno
Phone: (202) 586-7543
E-mail: charles.russomanno@ee.doe.gov
http://www.oit.doe.gov/forest/stability.shtml

Glass

Sensor Fusion for Intelligent Process Control
Gideon Varga
Phone: (202) 586-0082
E-mail: gideon.varga@ee.doe.gov
http://www.oit.doe.gov/factsheets/sens_cont/pdf/fact-fusion.pdf

Appendix B: OIT Contact Information

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Appendix C: Key Publications

CHEMICAL INDUSTRY VISION

Chemical industry leaders articulated a long-term vision for the industry, its markets, and its technology in the groundbreaking 1996 document *Technology Vision 2020 — The U.S. Chemical Industry*.

For more information, see http://www.chemicalvision2020.org

ROADMAPS FOR A COMPLEX INDUSTRY

Industry leaders developed technology roadmaps in diverse, critical areas. Roadmaps identify the priorities and performance targets for the chemical industry. They are used to identify opportunities for industry collaboration and to guide Federal R&D spending.

Completed roadmaps include:

- Biocatalysis (2000)
- Combinatorial Chemistry (2001)
- Computational Chemistry (1999)
- Computational Fluid Dynamics (1999)
- Materials of Construction (1998)
- Materials Technology (2000)
- New Process Chemistry (2001)
- Reaction Engineering (2001)
- Separations (2000)

Completed IOF roadmaps.

The following reports identify industry priorities that are useful in roadmap development:

- Alternative Media, Conditions, and Raw Materials (1999)
- Catalysis (1998)
- Process Measurement and Control: Industry Needs (1999)

For more information, see http://www.chemicalvision2020.org

ENERGY AND ENVIRONMENTAL PROFILE OF THE CHEMICAL INDUSTRY
DOE/OIT, 2000

This report takes a comprehensive look at the industry and identifies energy use for a wide number of individual processes, including ethylene, propylene, and agricultural chemical production, as well as the production of benzene, toluene, and zylene. It also presents an overview of the chlor-alkali industry and details the supporting process of effluent treatment and the use of process heaters.

For more information, see http://www.oit.doe.gov/chemicals

PILOT STUDY OF ENERGY PERFORMANCE LEVELS FOR THE U.S. CHEMICAL INDUSTRY
DOE/OIT, draft in publication

IOF has partnered with AIChE to develop and implement tools and methodologies that will drive improvements in operational efficiency as a means of meeting the chemical industry's energy reduction goals. These tools and methodologies assist funding agencies, company management, and engineering staff in evaluating the usefulness of potential process development and improvement efforts, tracking progress toward performance targets, and facilitating meaningful comparisons of energy use across the chemical industry.

Additional information is available at the following Web site: http://www.aiche.org/cwrt/practical.htm

MEASURING UP: RESEARCH & DEVELOPMENT COUNTS IN THE CHEMICAL INDUSTRY
Council for Chemical Research, 2001

The CCR report, *Measuring Up: Research & Development Count in the Chemical Industry*, quanitifies the critical role of R&D to the chemical industry for the first time. With economic, biometric, and historical analysis, this study shows how R&D has helped the chemical industry become a major building block of the U.S. economy and a world leader in scientific advances even in the face of increasing global competition.

Key findings of this new study include:

- On average, every dollar invested in chemical R&D today produces $2 in corporate operating income over a six year period
- Average annual return of 17% after taxes
- Business performs better when public policy, including government funding of R&D, is consistent
- Publicly funded science makes significant contributions to new technologies in the chemical industry

For more information, see: http://www.ccrhq.org/news/study_purchase.htm

OIT's Chemical IOF Team is responsible for managing the portfolio and pursuing activities to bolster the Chemical IOF.

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U.S. Department of Energy