Chemical Industry

VISION2020

Technology Partnership

An Opportunity for Chemical Companies

What is Vision 2020?

- Industry-led **partnership** — public and private
- On-going collaborative **process** to foster technology innovation

Goal: Leverage independent resources to identify and develop critical enabling technology

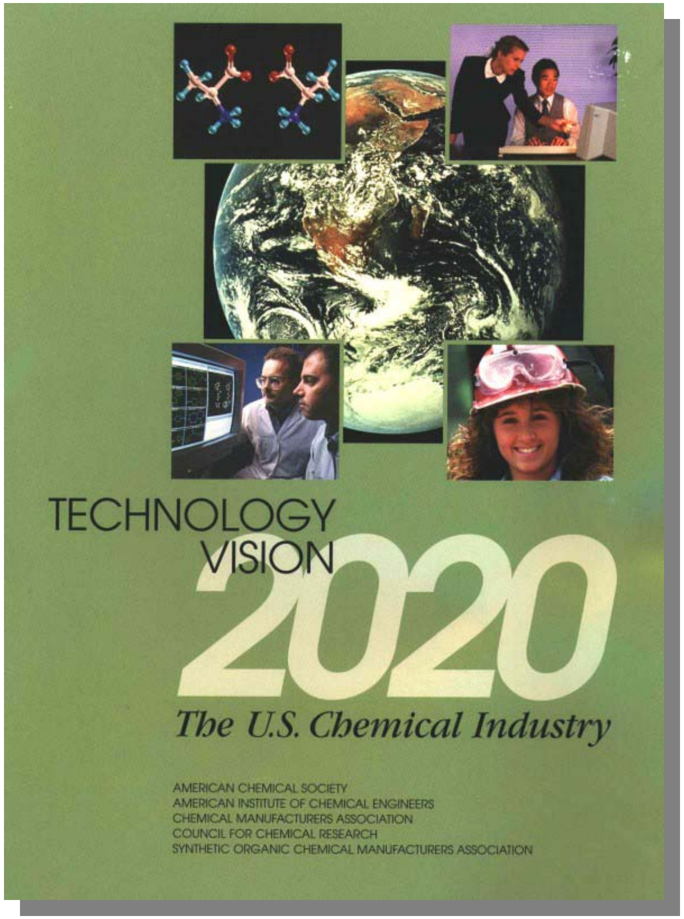
Vision 2020 Fits the Times

- Greater pressures on chemical company leadership
- Future growth, profitability, competitiveness, and long-term sustainability require new technology and business models for innovation
- R&D self-sufficiency is no longer realistic
- Public R&D investment should respond to industry needs
- Collaboration leverages resources and spreads risk

Vision 2020 Partners

Technology Vision 2020 —1996

- Consensus activity of 300 industry leaders
- Meeting challenges of the future requires
  - **New Technology**
    - Chemical Science & Engineering
    - Supply chain management
    - Information Systems
    - Manufacturing & operations
  - **Collaboration**
- Led to process detailing R&D needs and funding



From Vision to Reality

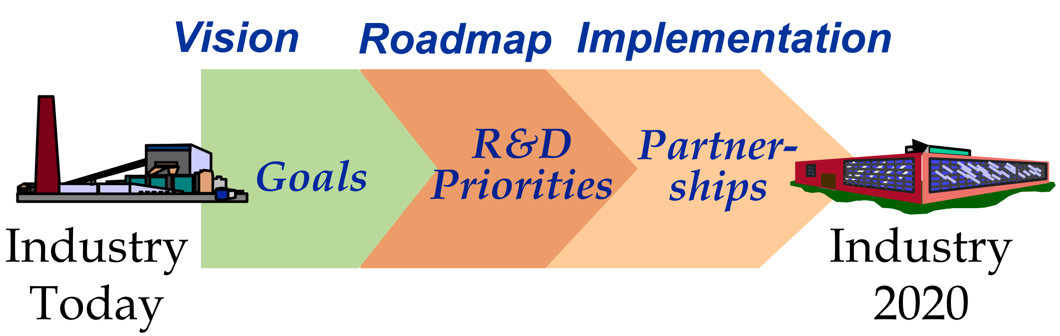
Vision 2020 Workshops Completed

- Catalysis
- Biocatalysis
- Alternative Reaction Conditions
- Alternative Reaction Media
- Alternative Raw Materials
- Combinatorial Chemistry
- Computational Chemistry
- Materials (I,II)
- Alternative Polymer Processing
- Chemical Analysis
- Separations (I,II,III, IV)
- Process Control Measurements
- Process Simulation
- Computational Fluid Dynamics
- New Process Engineering
- Reaction Engineering
- Manufacturing and Operations
- Agile Manufacturing
- Supply Chain Management
- Materials of Construction

New **Nanotechnology – October 2002**

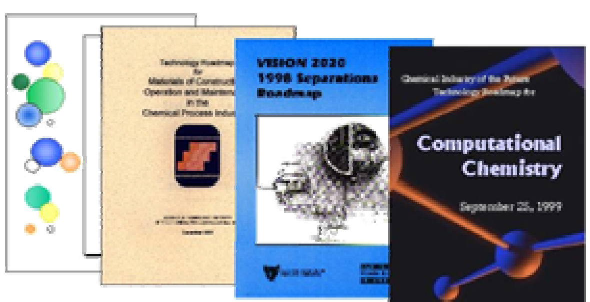
A Roadmap — Framework for Action

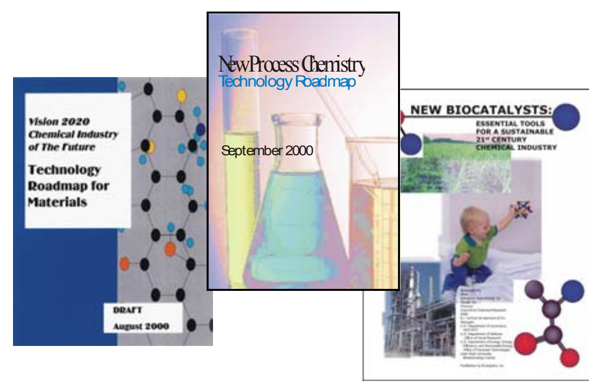
- Projects future needs
- Builds consensus among stakeholders
- Guides strategic choices for technology innovation
- Provides a practical tool and chronological path to get "from here to there"
  - Current State
  - Future State
  - Goals
  - Technical Barriers
  - Priority R&D Needs



Vision 2020 Roadmaps Completed

- Biocatalysis
- Combinatorial Chemistry
- Computational Chemistry
- Computational Fluid Dynamics
- Materials of Construction
- Materials Technology
- New Process Chemistry
- Reaction Engineering
- Separations
- Measurements for Process Control
- **Nanotechnology (review draft)**





Vision 2020 Web Site

http://www.chemicalvision2020.org

VISION2020 Members

Companies

Air Products *
BP
Cargill
Ciba Specialty Chemicals *
Degussa-Huls
Dow Chemical *
Dow Corning
DuPont *
General Electric
Millennium Corp
Praxair *
Rohm Haas *

Professional Associations

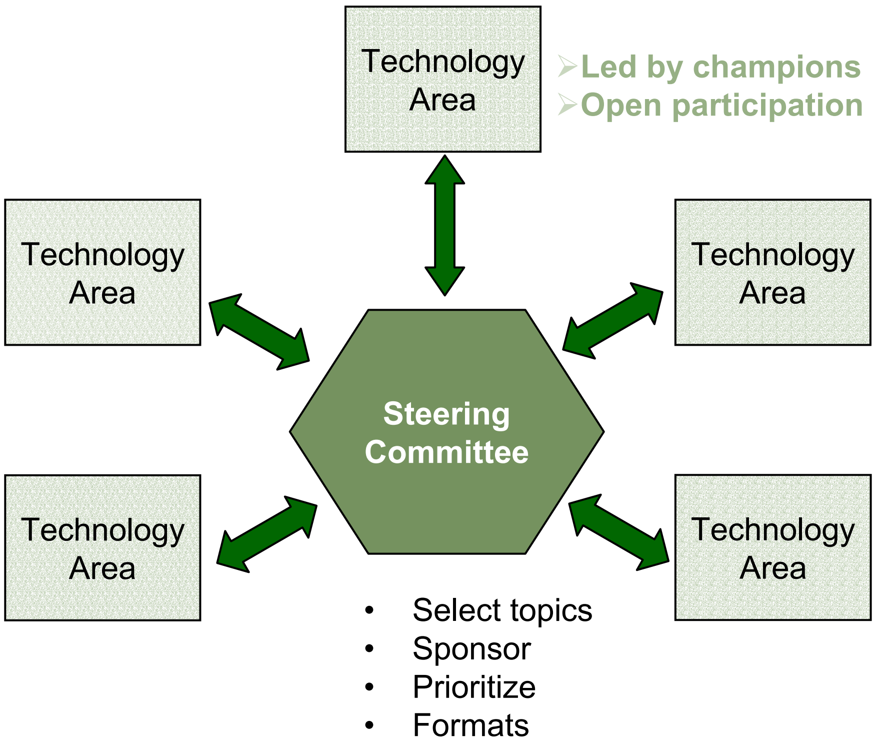
American Chemical Society
American Institute of Chemical Engineers - CWRT
Council for Chemical Research
Materials Technology Institute

VISION2020 Model

Steering Committee: plans, coordinates, prioritizes, and initiate activities for the benefit of all stakeholders - industry, academic, and public.

Technology Champions: formulate and drive specific project activity

ChemPlus (DOE/OIT) helps kick-start some projects by providing funds for background and scope studies



New Innovative Energy Systems Challenge

Vision2020 Technology Subcommittee

- Identify technology areas for R&D collaborations in pre-competitive areas that will result in widespread implementation of continuous improvement and/or breakthrough technologies to help enhance the competitiveness of the chemical industry and meet societal needs

- Facilitate formation of teams, or consortia, to implement industry-wide R&D collaborations
  - Industry,including medium and small businesses
  - National Laboratories
  - Academia

VISION2020 Technology Subcommittee

Technology Focus Areas

- Energy Efficiency and Renewable Energy - John Carberry, DuPont
  - Biomass to Energy - John Carberry, DuPont
  - Benchmarking & Evaluating Energy Efficiency - Jo Rogers, AIChE/CWRT
- Computational Methods
  - Physical and Chemical Properties - Tyler Thompson, Dow
- Advanced Separations
  - Bioseparations - Francis Via, Fairfield Resources
- Nanotechnology – Jack Solomon New

Nanotechnology: A New Vision2020 Focus Area

- Opportunities to leverage resources for nanotechnology development were tracked for 2 years
- National Nanotechnology Initiative (NNI) requested a roadmap (Jim Murday)
- Vision2020 rallied chemical company participation in planning workshop

NNI Grand Challenges

- **Nanostructured Materials by Design**
- Nanoelectric, Photonic, Magnetic
- Advanced Healthcare/Therapeutics
- Enivironmental Improvement
- Energy Conversion/Storage
- Microcraft & Robotics
- Chemical-Biological-Radioactive-Explosive Detection and Protection
- Instrumentation & Metrology
- Manufacturing Science

Vision for Nanomaterials by Design

Establish a "library" of diverse nanomaterial building blocks (less than 100 nanometers) synthesized by well-defined, economically viable manufacturing processes that display well-characterized compositions, stable architectures, and reproducible "properties."

These materials can be safely assembled using reproducible, cost-effective procedures into systems and devices that perform specified functions.

Nanotechnology Focus Area

Focus Area: **Nanomaterials for the Chemical Industry**

Project Leader: **Jack Solomon**

Partners: Air Products, Ciba, General Electric, Dow, Dupont, Praxair, Rohm and Haas

Status: Roadmapping workshop held Sept 30 – Oct 2

Goal: Define nanomaterials/nanotechnology R&D priorities for the chemical and material processing industry to guide government's multi-agency $750M/yr R&D effort

Sponsors: DOE (Materials and Chemicals), National Nanotechnology Initiative, Vision2020

Workshop Planning Committee

- Air Products - *Frank DiStefano*
- Dow Chemical - *Susan Babinec, Paul O'Connor*
- Dupont - *Rajeev Gorowara*
- General Electric - *Judith Stein*
- Oak Ridge National Lab - *Sharon Robinson*
- Praxair - *Frank Notaro, Jack Solomon*
- Rohm and Haas - *Catherine Hunt, Frank Lipiecki*
- US Naval Research Lab - *Jim Murday*

Nanotechnology Workshop

- **Workshop participants**
  - 95 people from industry (60%), academia (15%) and government (25%), including 9 agencies and the White House
    (AIChE participants: Gil Lee and Mathew Tirrell)
- **Workshop format**
  - **Materials**
    - Nanomaterials
    - Dispersions & Nanocomposites
    - Ordered Nanostructures
  - **Enabling Technologies**
    - Analytical Tools
    - Simulation/Modeling
    - Manufacturing
  - **Integration/Cross-Cutting**

Nanotechnology Workshop & Roadmap

Desired Outcomes

- Key trends and opportunities; quick wins
- Technical challenges and barriers
- Prioritized R&D needs
  - Expected timeframes for completing activities (near-, mid-, and long-term), outcomes and interrelationships
  - Potential funding agencies
  - Possible industry-academia-government partnerships
- Identify possible quick wins

Nanomaterials

(Frank Notaro – Praxair)

- Develop capability to determine application enabling properties (modeling, synthesis, characterization & functional testing)
- Develop capability to predict and control enabling properties (Modeling, synthesis & characterization)
- Expand the type and number of organic and inorganic nanomaterial building blocks to enable new applications
- Develop and incorporate self assembly capability at the interface of building blocks
- Develop nano-matter building blocks that enable self repair of coating structures at the micron to millimeter level

Dispersions and Nanocomposites
(Paul O'Connor - Dow Chemical Company)

- Surface Chemistry & Interfacial Control
  - Develop Surface Functionalization Methodologies
  - Better fundamental understanding of the role and control of interface
- Theory & Modeling
  - Length-scale bridging of modeling NC
  - A predictive toolbox for NC properties
- Characterization
  - Methods to determine degree of dispersion
  - Measuring interface properties
- Manufacturing Fundamentals
  - Techniques for nano-scale separation & classification of nano-particle dispersions

Ordered Nanostructures

(Judith Stein - General Electric Company)

- New paradigms for useful building blocks based on thermodynamic and kinetic rules for ordered nanostructures
- Directed self-assembly techniques and new methods of high fidelity top-down assembly for ordered nanostructures that can provide short to long-range order.
- Tools to predict and measure properties at the highest resolution possible in space and time for ordered nanostructures. Utilization of tools at national facilities
- Standard methods, materials and codes for nanometrology (with emphasis on ordered nanostructures)
- Processing technology leading to manufacturing capability for ordered nanostructures
- Real, useful, and novel applications of ordered nanomaterials that exploit unique nanoscale properties
- Computational models and schemes for predicting properties at nano and across length scales for ordered nanostructures

Analytical Tools

(Catherine Hunt – Rohm & Haas)

- Structure/Property relationships between **Nano and Macro Worlds.**
- **Enhanced Resolution** for all characterization tools.
- Close coupling between **Theory/modeling and Experiment.**
- Develop tools that are capable of nano analysis of **bio-systems.**
- Improved tools for analysis of **buried interfaces.**
- Tools for **high throughput** analysis and to enable **"real time"** analysis.
- Improved nano-chemical contrast coupling **structure and function.**

Modeling/Simulation and Informatics

(Rajeev L. Gorowara - E.I. du Pont de Nemours and Company)

- Accurate predictive models
  - linking nano-scale properties across time and length scales to specific macroscopic properties
- Other technical goals
  - Model the formation process; predict new properties; manage the information
- Develop methods for including chemistry (rxn & degradation) in force field models.
  - Model chemistry of deformable interfaces, e.g. during production of nano-structures
  - Integrate chemical functionality of nano-structure into models
- Bridge modeling between scales (from atoms to self-assembly to devices)

Manufacturing
(Frank Lipiecki – Rohm & Haas)

- Manufacturing processes important to produce brand new products with advanced properties (scaling, process monitoring & control)
- Manufacturing model similar to traditional models, yet need for novel concepts evident
  - In unit processes
  - New ways to put thing together (biological, self-assembly)
- Material characterization, Structure-Property relationships must be established

CROSS-CUTTING

- Shift emphasis away from discovery to applied R&D and commercialization (SBIR Phase 3)
- **Health/Safety/Environmental aspects need to be addressed**
- Develop a Common "Language" for nanotechnology practitioners (Nomenclature,Definitions, Glossary of terms)
- Continue to foster collaboration among industry, government, universities on manufacturing issues
- Develop "resource centers" (standards for characterization, databases, models, informatics, etc.)
- Much can be done pre-competitive
- Shape public opinion

Early Wins: Catalysts, Coatings, Optical and Electronic Displays

Next Steps: Nanomaterials Roadmap

- Publish strategic R&D roadmap in early 2003
- Leverage financial and technical resources to accelerate R&D
- New SBIR and STTR solicitation includes 2 technical topics – *due Jan. 14, 2003*
  - Nanotechnology applications in industrial chemistry
  - Nanomaterials for energy efficiency

http://sbir.er.doe.gov/sbir/