Planning Report 09-1

Retrospective Economic Impact Assessment of the NIST Combinatorial Methods Center

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RTI International
for

National Institute of
Standards & Technology

April 2009

National Institute of
Standards and Technology
U.S. Department of Commerce

April 2009

Retrospective Economic Impact Assessment of the NIST Combinatorial Methods Center

Final Report

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EXECUTIVE SUMMARY

The National Institute for Standards and Technology (NIST) launched the NIST Combinatorial Methods Center (NCMC) in 2002 to develop and transfer to industry and academia technology that would assist researchers in significantly increasing the efficiency of their polymers research programs. Materials research is the basis for a wide range of polymer-related product (e.g., plastics, coatings, formulations), which, in turn, drive the global supply chain for a wide range of final goods and services.

Given this critical role, technology infrastructure that makes R&D processes more effective and efficient and that enables the discovery of enhanced materials has the potential to improve economic, environmental, and public health welfare. Increasing research output per dollar of input, shrinking development times, and avoiding needless research in the upstream portion of the product supply chain hasten the introduction of new products and the benefits these products offer consumers over their predecessors.

Combinatorial methods, referred to collectively as “combi”, offer scientists an alternative to manual “one-at-a-time” research techniques for discovering new materials. They enable the creation of a large number of related chemical samples (known as libraries) and the rapid analysis of those samples’ properties, known as “high-throughput screening” or “high-throughput experimentation”.

In its initial foray into combi for polymers, NIST developed a simple but elegant approach for studying and screening new material compounds. The provision of continuous gradient libraries enabled researchers to vary material thickness and processing temperature, for example, on a substrate, and then analyze the entire gradient for combinations of interest at one time instead of preparing and analyzing individual samples.

The acclaim that the results from this research received coupled with the stated needs from industry and academia for a community dedicated to combi provided the rationale for NIST to launch the NCMC, a public–private research consortium dedicated to combi’s development.

ES.1 NIST’s Objectives for the NIST Combinatorial Methods Center

Three overarching objectives characterized the NCMC when it was launched:

- Provide technology to overcome technical barriers to combinatorial and high-throughput experimentation for organic polymers.
- Disseminate research findings rapidly, offer instruction and best practices, and proactively engage the materials science community to raise awareness of the advantages of combinatorial and high-throughput experimentation for materials discovery.

- Establish a forum wherein NIST, industry, and academics could exchange ideas and techniques, identify technology needs, and set research needs.

The NCMC was conceived as an "open-source" community supported by NIST and industry members' annual fees. All NCMC innovations enter the public domain. The Center offers novel technology solutions that minimize costs and maximize throughput and information capture. The NCMC adopted a consortium model to maximize technology transfer from the NCMC to industry and academia. NIST supports this transfer-efficiency objective by releasing tools, data, and methods as they are developed. Strategic planning is also enhanced by industry participation in the consortium, which assists NIST in ensuring that the optimal portfolio of infratechnologies is developed in response to industry's needs.

The NCMC has also become a nucleus for coordinating and driving symposia and national and international meetings, the interface with the American Chemistry Society (ACS) and the Materials Research Society (MRS), and interactions with other leading professional associations for materials science.

As an additional output from its efforts, the NCMC has published more than 60 papers in the science and technology literature.

In addition, the NCMC has

- sponsored more than 20 sessions and conferences nationally and internationally about advances in combi for polymers,
- hosted researchers for over 455 training days at NIST between 2002 and 2007,
- trained more than 25 new experts in combi through its postdoctoral research program,
- organized 14 semiannual meetings with presentations, technology demonstrations, and round-table discussions of technology infrastructure advances and needs, and
- presented more than 200 invited talks at key international meetings, industry sites, workshops, and universities, including Gordon Research Conferences, ACS,MRS, GE, 3M, PPG, Bayer, IBM, Dow, Air Products, BASF, MIT, and Cornell.

In late 2007, NIST contracted with RTI International to perform a retrospective economic impact assessment of NIST's activities from the launch of its pilot continuous gradients project in 1998 through 2007. The study's goal was to quantify economic impacts, assess the effectiveness of the consortium approach, and chart the NCMC's influence in encouraging and accelerating the introduction of combi for polymers.

ES.1 NCMC's Contributions to Combi for Polymers R&D

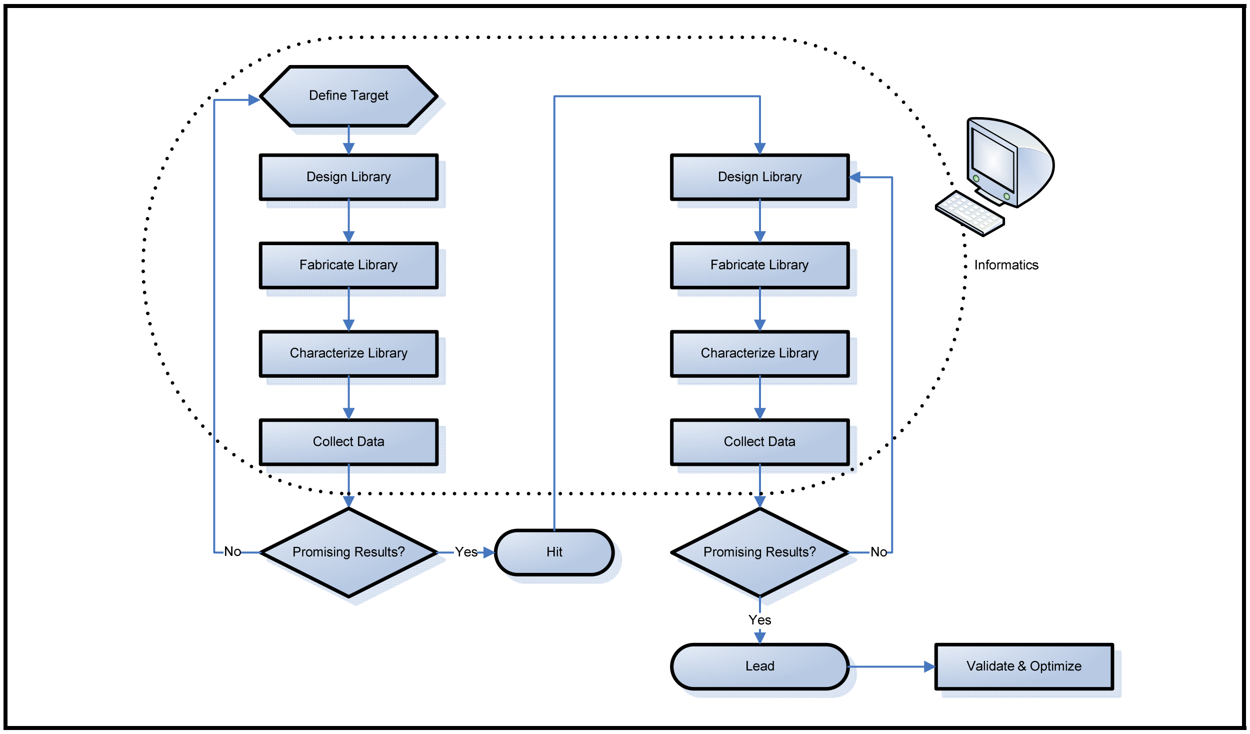
The three characteristics of materials discovery—that materials are tailored for specific applications, that materials are formulated from many components, and that each component has a structure and intricate behavior—are the root of the challenge of using combinatorial approaches for materials.

In recent years, property specifications for materials mandated by end users have simultaneously increased and become more complex. The increasing difficulty in developing new materials led Bayer Materials Science (a NCMC member organization) to declare that a “revolution” was needed in coatings science, and this “revolution” would be provided in the form of combinatorial methods (Wicks and Bach, 2002).

Combi can improve each stage of the experimentation cycle to create a seamless “combinatorial workflow” process (see Figure ES-1). Screening a fabricated library rarely presents researchers with a simple yes/no answer. Because typically more than one property is of interest and because material properties are a continuum of values (versus discrete reacts or does not react), the set of desired properties may be physically or chemically incompatible. Materials scientists must make trade-offs between properties such as hard (high modulus) yet brittle (low strength) versus soft but elastic. Combi and materials R&D in industry is a continuum of phases starting with discovery, transitioning to optimization, and ending with a product.

Building a high-throughput workflow based on robotics is capital intensive, requiring start-up investments ranging between $8 and $20 million (Symyx, 1999). An Advanced Technology Program (ATP) white paper published in 2000 argued that “discontinuous innovation in generic and/or modular hardware and software technologies will be necessary to drive down costs and facilitate its implementation in industrial sectors that have lower returns on R&D investment, such as exist in the chemical and materials industries” (Hewes, 2000).

Figure ES-1. Combinatorial Workflow Cycle
A robust combinatorial system for materials research includes an informatics system to handle data and guides the research process.



The NCMC made significant contributions to the development of less-expensive research capital and supporting technology infrastructure for the fabrication and testing of combi polymer libraries, thereby reducing costs associated with the application of combi methods to polymer materials research and stimulating U.S. industry to adopt combi and think innovatively about applying the concept of combi to polymers research.

In summary, using NCMC's approaches, researchers are able to rapidly map out structure–property relationships in systems with multiple parameters. This enables developers to more rapidly and efficiently develop new materials, optimize a material for a particular application, and respond more quickly to changes in the prices of raw materials and market demand. Additional benefits may include reduction in materials consumed and waste generated while developing a new polymer material because of reduced sample size and development of more robust materials because of the ability to test over a much broader range of conditions or explore a larger combination of components.

With respect to scope of impact, NCMC's work touched on each phase of the combi workflow and three different platforms for library creation: gradient thin films, discrete libraries created by robotic dispensing systems, and microfluidics. Testing of polymer libraries frequently requires new or modified equipment to speed up the measurement process creatively. As summarized in Table ES-1, NCMC innovated more than six measurement methods and made contributions to several more for library measurement. By design, combi generates large volumes of data that have to be captured, processed, and reported in a meaningful manner. This informatics aspect of combi was also a research area for the NCMC.

NCMC advances were particularly important to key economic stakeholders active in polymers R&D:

- advanced materials manufacturers (e.g., resins, rubber, specialty chemicals, synthetic fibers) that produce and market material components to other industrial consumers;
- paints, coatings, and adhesives manufacturers (collectively referred to as "coatings");
- personal care and household products firms that use combi to study formulations;
- academic and government laboratories that employ combi in academic research settings; and
- laboratory equipment, software, and service providers that participate in the consortium to connect with customers, participate in the technical dialog, and leverage NCMC's methods, software, concepts, and manuals.

In the views of interviewees in these sectors, equally as important to NCMC's technical accomplishments are the NCMC's contributions to the development of human capital and a technical community focused on combi. Human capital development consists largely of NCMC postdocs who offer industry and academia talented, multidisciplinary researchers and host researchers from NCMC member organizations and international standards bodies. A significant proportion of the Center's mission has been focused on outreach, and the NCMC organized and led symposia at MRS and ACS meetings, among others, that demonstrated the possibilities with combi to large numbers of researchers.

Organizing tracks and symposia at major MRS and ACS conferences as well as at more targeted audiences for Knowledge Foundation and Gordon Conference meetings have offered the staff access to audiences outside of the immediate membership. Indeed, the NIST staff and their projects were central to starting the Gordon Conference series on combi. Certainly, the staff maintain professional relationships with other researchers, but organizing symposia offered the Center the opportunity to present formally and provide evidence of the consortium's technical accomplishments.

ES.3 Methodology for Estimating Economic Benefits of the NCMC

Our approach to valuing economic impacts was to prepare a series of counterfactual analyses that linked hypotheses about the NCMC's benefits to relevant technical and economic metrics. These metrics then informed processes for collecting data and estimating measures of economic benefit. Benefits were estimated against a scenario in which the NCMC did not exist and key advances in thin films and microfluidics libraries were not made.

Table ES-1. NCMC Platforms for Library Creation

Platform and Library Properties	NIST Original
Gradient thin film libraries for polymers	
Thickness gradient	Yes
Surface energy gradient (UV ozone)	Yes
Temperature gradient	Yes
Composition gradient	Yes
Graded chemically patterned substrates	Yes
Discrete sample libraries	
Composition gradients for solutions	
Composition gradients for films and "dots" (blobs of polymer)	
Temperature gradient in position or time	
Microfluidics libraries	
Composition gradients, discrete library by droplet	
Composition gradients with reaction in organics, discrete library by droplet	Yes
Solution-deposited films (brushes) with chemical/composition gradient, continuous sample (film)	Yes
Solution-deposited copolymer films with chemical/thickness gradient, continuous sample (film)	Yes

The total economic impacts of infratechnology development and consortium programs such as the NCMC can be broken out into five distinct categories:

- *technology adoption/adaption*: the benefits of adopting new technologies or adapting them to suit an organization's purpose
- *knowledge base expansion*: the benefits of acquiring technical information and data that improve an organization's knowledge base
- *consortium experience*: the benefits of membership in narrowly defined forums in which all respondents are focused on a single technical topic
- *downstream product cost and quality*: improved quality of goods and services in which those materials are an input and that potentially reduce the costs of those goods and services
- *time acceleration effects*: accelerated the accrual of cost savings or product quality benefits for end users

The first three bullets pertain to R&D efficiency: acquiring infratechnology and knowledge that permit researchers to do more with less. NCMC methods and "how-to's" for adapting common laboratory apparatus to enable them to perform high-throughput experiments and to enable end users to accrue labor, material, and capital cost savings over the life of the project, relative to the defending manual one-at-a-time methods.

In economic analyses such as this one, each component of the total economic impact will generally have elements that are more tangible than others. For example, stakeholders could not quantify downstream product quality benefits or end-user acceleration benefits. Quantification is very difficult, although it is likely that benefits do exist.

Today some research laboratories are using combi that otherwise would not because of NIST's program. NIST's contributions to microfluidics and thin-films research were particularly significant with respect to impact. Symyx and other vendors were offering comparable and, in some cases, more sophisticated technologies for discrete sample libraries, but NIST was the leader in thin films and microfluidics for polymers. Interviewees believe it would have taken from 5 to 10 years before comparable, inexpensive infratechnologies for thin films would have been devised without NIST's contribution.

The counterfactual scenario against which benefits were measured specified that

- the novel suite of techniques for gradient approaches to thin films and elements of microfluidics and discrete sample library combi would not have been available before 2008 and firms would have incurred greater capital, materials, and labor expenses as a consequence;
- the overall adoption rate of combi for organic polymers would have been lower, meaning that some users' adoption likely would not have occurred until years later;

- the costs of adopting combi would have been higher, and some laboratories would not have been using combi at all; and
- the absence of the NCMC would have hampered information diffusion and offered no coordinated forums for discussion of the development of the combi toolkit for organic polymers, particularly for thin films and microfluidics.

Data informing this analysis were collected from semistructured interviews, survey forms completed via e-mail and returned to RTI, and an Internet survey of materials discovery scientists. Most responding scientists were employed by NCMC members or alumni, research universities, or large chemical companies that did not join the NCMC. All were directly involved in polymers R&D.

Results from the survey sample were extrapolated to national estimates using publicly reported R&D expenditures for firms in the advanced materials, paints and coatings, and personal and household care product industries that are likely to be using combinatorial methods in their research.

ES.4 Net Economic Benefit Estimates

ES.4.1 Economic Benefits of Consortium Experience

The consortium offered valuable demonstration and training opportunities that enabled companies to keep more readily abreast of the latest in combi-related research. They were also able to acquire information on novel approaches and inexpensive strategies for incorporating them into their workflows (see Table ES-2).

On an annualized basis, 78% of members and alumni stated that the benefit of participating was equal to or greater than the membership fees paid. Half indicated that the NCMC validated internal research strategies or invalidated strategies that would not have born fruit. A former NCMC member commented that “the greatest benefit NCMC provided was a regular forum for combi materials … which helped provide technology and competitive awareness [as well as] discussion and networking opportunities within the combi materials community.”

Another member noted that “the biggest benefit we have gained from NCMC is the ability to see the internals of complete ‘combi’ procedures, not just the finished product. So, by being a member of NCMC we have been able to see a project being defined, problems being identified and solutions being developed—equally the handling of samples and information from the beginning to the end of an experimental process—unlike the snapshots seen via commercial interactions.”

Table ES-2. NCMC Members' Perceptions of the Benefits of Membership

Survey Question	Yes	No
Was the annual benefit your organization accrued from participation in the NCMC equal to or greater than the annual membership fees paid?	78%	22%
Did participation in the NCMC … offer more productive marketing or networking opportunities, relative to other conferences or combi meetings?	83%	17%
… validate or invalidate internal research projects and permit more efficient and effective resource allocation?	50%	50%
… help your organization avoid any research activities, or enable your organization to acquire needed research more quickly or cost-effectively?	70%	30%
… offer valuable researcher training and demonstrations beyond what would have been available elsewhere?	67%	33%

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

ES.4.2 Economic Benefits of Knowledge Base Expansion

The second component of estimated economic benefits was NCMC's contributions to the expansion of the body of knowledge essential to implementing and using combinatorial approaches. Data provided by respondents indicate that the economic benefit of NCMC's contributions to the combi knowledge base totaled nearly $24.4 million over the period from 2001 to 2007 (see Table ES-3).

These information acquisition benefits reflect two distinct advantages that accrued to end users. First, NCMC's papers and presentations invalidated some firms' research strategies, enabling them to avoid expending resources on projects that either would have ultimately failed or that would not have been as effective and efficient as those the NCMC published. Second, respondents stated that they acquired valuable knowledge about combi in general and about specific approaches.

One researcher noted that although his lab had not implemented any of the methods developed by the NCMC, the overall body of knowledge that the consortium generated offered valuable insights into implementing and employing combinatorial approaches.

ES.4.3 Economic Benefits of Technology Adoption and Acceleration

The final component of economic benefits was the benefit of adopting NCMC combi technology and the economic benefit from accelerating firms' combi adoption. In the case of methods developed by NCMC, the study valued the introduction of novel technology that otherwise would not have been introduced within this study's period of analysis.

Table ES-3. Respondents' Adoption and Awareness of NCMC Combi Technology

Respondents' Use of the Following Methods and Technologies Developed by the NCMC and its Industry Members (% of respondents):	Use or Adapted	Aware of but Not Relevant	Unaware of Technology
Continuous thin films with gradients in temperature, composition, thickness, surface energy, or on chemically patterned substrates	45%	55%	0%
Discrete libraries used with gradients in temperature, surface energy, or thickness	32%	55%	5%
High-throughput measurement of morphology	27%	41%	23%
Buckling method of modulus measurement for thin films and soft materials	23%	64%	9%
Edge lift-off test for interfacial adhesion	23%	64%	9%
Microfluidics produced organic solvent-based libraries	14%	64%	14%
Multilens contact test for adhesion	5%	77%	9%
Interfacial tension measurement via microfluidics	5%	77%	9%
Integrated metrology (morphology, composition, extent of reaction) on microfluidics produced organic solvent-based libraries	0%	73%	18%

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" survey.

Some firms also reported accruing benefits due to accelerated adoption attributable to the NCMC. R&D efficiency benefits accrued to firms who adopted combi earlier than they would have in the absence of NCMC's industry outreach work and publications. Where firms reported that their adoption of combi was accelerated, the firms' net benefits from the acceleration effect were included in the benefits estimate.

First, economic benefits from adopting NCMC-developed technology were quantified by measuring the cost savings from using NCMC approaches rather than the next best alternative ("defending") method. Productivity gains were defined as increases in the number of equivalent samples analyzed per day per researcher. Economic benefits were the value of the increase in throughput and the volume of information acquired for equivalent or lower labor, materials, or capital expenditures.

As illustrations of how NCMC's research generated economic benefits:

- One researcher told us that without NCMC-developed approaches her company would not have undertaken what proved to be a highly successful project because it would have taken 10 times longer and have been 10 times more expensive.
- Another indicated that using NCMC's temperature gradient approach she can accomplish in 30 minutes what would have otherwise taken her 375 minutes.
- One firm credited NCMC's research with assisting in the development of advanced formulation systems used in their coatings research. The formulation system was

installed in each of the firms' R&D labs, and they estimate savings to date of several million dollars compared to the cost if they had installed commercially available formulators.

- The work performed by NCMC on microfluidics for measuring interfacial tension helped another firm develop its own microfluidic equipment. This equipment enabled its lab to perform tests up to 3 times faster compared to the previous method while using fewer materials. Working with smaller samples had an important environmental benefit because the smaller samples size reduced waste, which, in turn, reduced hazardous material disposal costs.
- The edge lift-off test for interfacial adhesion was credited for enabling another firm to analyze 5 times more combinations of parameters than had been possible with previous methods. Although this firm did not cite significant gains in throughput, the method did permit them to study their samples more thoroughly. As a consequence, the firm believes that their customers have more robust products.

Over 90% of respondents reported that the NCMC technologies offered efficiency benefits over the technologies that they had been using before, and a slightly higher percentage reported that these technologies also enabled them to test across a broader range of samples. NCMC technology also improved the effectiveness of their R&D: 92% of respondents stated that NCMC technology improved the quality of their research and/or products that their company may produce.

Table ES-4 presents the average reported labor productivity gains for using combi in polymers R&D in general and for using the NCMC-developed technology. The mean labor productivity gain reported from combi overall (i.e., not from only NCMC approaches) was about 8.5 fold, with individual responses ranging between 1.5 and 24 fold. Driving this overall productivity gain estimate is the gains from NCMC-developed technology.

The mean reported labor productivity gain for NCMC-developed approaches was 5.2 fold, with individual responses ranging between 1.2 and 12.5 fold. Follow-up interviews to explore the wide variation in reported gains suggested that the variation was attributable to differences in the techniques applied by various labs, properties of targeted materials, and required rate of automation, for example.

Table ES-4. NCMC Acceleration of and Estimated Productivity Gain from Combi

Measure	Value
Mean overall net labor productivity gain from using combi for polymers R&D, where applicable	8.5 fold (Range: 1.5 to 24 fold)
Mean reported net labor productivity gain from using NCMC-developed technologies for polymers R&D, where applicable	5.2 fold (Range: 1.2 to 12.5 fold)
Percentage of respondents reporting that NCMC accelerated their adoption of combi for polymers R&D	50%
Mean number of years respondents reported that NCMC accelerated their combi adoption	2.3 years (Range: 1 to 5 years)

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" survey.

Half of all respondents reported that NCMC an accelerated their adoption of combi. The average adoption acceleration was 2.3 years. Some reported that their adoption of combi was accelerated by 4 or 5 years. A recurring theme was that interaction with NIST researchers gave firms more confidence in their decision to proceed with investments in combi programs.

The publicity and attention NCMC drew to combi made it easier for some researchers to convince senior executives within their organizations to invest in combinatorial approaches because NCMC and NIST demonstrated that a reputable institution had successfully performed combi for polymers.

ES.4.4 Net Economic Benefits

Table ES-5 assembles the complete time series of quantified costs and benefits for 1998 through 2007. Total benefits were estimated to be $210.4 million for the advanced materials, coatings, and personal and household care products industries:

- $1.1 million from adoption and demonstration benefits from participating in the consortium,
- $24.4 million from expanding the knowledge base supporting combi, leading to more informed combi R&D research project selection, and
- $184.8 million through product R&D efficiency realized from applying NCMC technology and through accelerating many firms adoption of combi and high-throughput research methods.

Total NIST costs from 1998 to 2007 were approximately $14.5 million. These costs were augmented by NCMC membership and focus project fees of around $1 million and technology acquisition costs for NCMC-developed technology of about $7.5 million, including capital and initial labor expenditures. Total costs were therefore about $23 million.

Inclusive of NIST, NCMC member, and technology acquisition costs net benefits were $187.4 million. The vast majority of benefits accrued from using NCMC-developed technologies, but the knowledge base expansion benefits equivalent to more than 10% of total benefits are certainly significant. These less tangible benefits are essentially a slice of the minimum alternative development cost for the technologies that NCMC developed for the equivalent of $23 million, and part of that $23 million included costs for administration and outreach work.

The net present value (NPV) of net benefits was $118.0 million applying the OMB-approved discount rate of 7% (see Table ES-6). The benefit-to-cost ratio, which is the ratio of the NPV of total benefits to that of costs, was estimated to be 8.55. In other words, for every $1 that NIST and its partners invested in the NCMC at least $8.55 in benefits accrued to the three industries.

The internal rate of return (IRR) was estimated to be 161%. Because the results of NCMC activities are widely used by many companies and other organizations, they have what economists call “public-good” content. In such cases, the IRR is called the “social rate of return”. Based on reviews of many economic studies, the hurdle rate for rationalizing such public-good investments is in the 30−50% range (Tassey, 2003). Thus, the NCMC returned at least three times what would be considered the minimum acceptable IRR.

Table ES-5. Net Quantified Economic Benefits of the NCMC

Year	Consortium Experience ($thousands)	Knowledge Base Expansion ($thousands)	Technology Adoption & Acceleration ($thousands)	Total Benefits ($thousands)	Total Costs ($thousands)	Net Benefits ($thousands)
1998					(286)	(286)
1999					(495)	(495)
2000					(556)	(556)
2001		103		103	(2,266)	(2,164)
2002	124	558	10,912	11,594	(2,535)	9,059
2003	294	4,768	31,349	36,411	(3,166)	33,245
2004	266	4,981	41,344	46,591	(3,409)	43,182
2005	151	4,806	37,366	42,323	(4,120)	38,203
2006	186	4,912	33,575	38,673	(3,806)	34,867
2007	113	4,306	30,293	34,713	(2,418)	32,295
Total	**$1,134**	**$24,434**	**$184,839**	**$210,408**	**(23,057)**	**$187,351**

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. Sums may not add to totals due to rounding.

Table ES-6. Performance Measures

Measure	Value (2007$)
Total quantified benefits	$210.4 million
Total quantified costs	$23.1 million
Net present value of net benefits (NPV) (Base year = 1998)	$118.0 million
Benefit-to-cost ratio (BCR)	8.55
Internal rate of return (IRR)	161%

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. NPV was calculated using the 7% real social discount rate recommended by OMB.

ES.5 Remarks on the Effectiveness of the Consortium Approach

Through the NCMC's work, researchers acquired both technology and evidence of how investments in combi could increase R&D efficiency and hasten the development of more robust polymeric materials and the products whose performance or quality is enabled by those materials.

The technology NCMC developed between 1998 and 2007 enabled organizations to reap significant R&D efficiency benefits by integrating and adapting for their use methods such as continuous gradient thin films, microfluidics libraries, and the edge lift-off test for interfacial adhesion. As a recognized leader in metrology, NIST assumed the role of filling technology gaps left unaddressed because of market and technical barriers. NIST was also able to leverage its reputation for scientific excellence and independence into a leadership role for the technical community.

If it were not for these attributes – leadership in metrology, impartiality, and a reputation for scientific excellence– the creation of a consortium like the NCMC as a precompetitive forum whose members were all from the private sector would have been highly unlikely. Beyond developing and then rapidly transferring technology into the public domain, NCMC's outreach work, research, and publications demonstrated what was possible with combi. The combination of these activities had a pronounced effect on industrial R&D efficiency—a critical factor in an increasingly technology-based global economy. The NCMC offers an excellent example of much of the best of what NIST has to offer in science & technology development and outreach:

- overcoming technology gaps through the development of infratechnology,
- convening researchers in independent, precompetitive forums to disseminate research and best practice,
- partnering with government and academia to develop and execute research projects of particular relevance to industry,

- demonstrating what is possible and advocating for novel approaches for rapidly identifying research foci, and
- championing the adoption and development of new approaches that offer R&D and production efficiency benefits as well as the opportunity to discover groundbreaking new materials.

In summary, the consortium model proved to be particularly effective. The results of this study provide evidence of how industry participation in the research program combined with government (NIST) support can allow a strategic focus on areas of systematic private-sector underinvestment, specifically generic technologies and infratechnologies essential to a technology's development and use. NIST benefited from industry's feedback, and industry benefited from access to information on a prepublication basis as well as from hands-on demonstrations of novel approaches. The feedback loop inherent in this approach integrated NIST's mandate to expand the frontier of measurement science with industry's desire for research outcomes to be relevant to their needs.

1. STUDY INTRODUCTION

The science of materials discovery and development is such a fundamental function within the global supply chain for goods and services that the question of what commodities and finished goods are *not* affected by it in some way becomes difficult to answer. In the modern economy, early in the planning stages of production emerge the critical questions of: From what materials shall a product be made? What criteria must those materials meet in order to be acceptable for the desired product? How can we enhance key materials' properties to improve the product's performance?

These questions compel U.S. industry to expend billions of dollars in research and development (R&D) annually on materials discovery, development, and optimization. The scale of materials R&D is so large because, by definition, materials are an intermediate good. Just as products are of a seemingly infinite variety, so too are the materials of which they are composed. The performance of a product purchased from a store shelf largely depends on the properties, characteristics, and interactions of its constituent compounds.

A large proportion of the value-added manufacturing sector consumes as inputs in their production processes the output of large materials, specialty chemicals, and coatings companies. Many vertically integrated firms and industrial conglomerates (e.g., General Electric, Procter & Gamble, and 3M) maintain research units that develop materials for use by sister companies and other divisions under their corporate umbrella. In addition to their counterparts within corporate R&D centers, research groups in academia and the public sector engage in basic and applied research to build the knowledge base of phenomena in materials and to develop novel materials to meet national priorities.

Given the critical role materials science plays in the economy, technology infrastructure that makes R&D processes more effective and efficient and that enables the discovery of enhanced materials has the potential to improve economic and environmental welfare. Increasing research output per dollar of input, shrinking development times, and avoiding needless research in the upstream portion of the product supply chain hasten the introduction of new products and the benefits these products offer consumers over their predecessors.

The National Institute for Standards and Technology (NIST) launched the NIST Combinatorial Methods Center (NCMC) in 2002 to develop and transfer to industry and academia technology that would assist researchers in significantly increasing the throughput of their research programs. Materials research in the key area of polymers (e.g., plastics, coatings, formulations) is a time-consuming and resource-intensive process. The pharmaceutical industry addressed the same throughput challenge via combinatorial chemistry—the systematic synthesis of a large variety of chemicals and screening the results for drug candidates. In theory, the same approach was possible for polymers science, but the reality was that the obstacles posed by polymeric materials were more challenging than those faced by the drug industry from chemicals suspended in purified water. Polymers are often viscous, solvent-based, and processed at high temperatures. The dearth of available research and technical expertise in high-throughput experimentation for polymers meant that even the most basic infrastructure for combinatorial methods in many applications was nonexistent. The same equipment employed by the pharmaceutical industry would be quickly destroyed by the industrial solvents and heat needed for polymers.

In its initial foray into combi for polymers NIST developed a simple but elegant approach to using combinatorial and high-throughput experimentation, collectively referred to as “combi,” for thin polymer films. The acclaim with which the results from that project were met coupled with the stated needs from industry and academia for a community dedicated to combi provided the rationale for NIST to launch the NCMC, a public–private research consortium dedicated to combi’s development.

In late 2007, NIST contracted with RTI International to perform a retrospective economic impact assessment of NIST’s activities from the launch of its pilot thin films project in 1998 through 2007. The study’s goal was to quantify economic impacts, assess the effectiveness of the consortium approach, and chart the NCMC’s influence in encouraging and accelerating the introduction of combi for polymers. This report is the study’s final deliverable.

This introductory chapter offers a foundational discussion on key subjects necessary for describing the NCMC’s scientific accomplishments and economic impacts. The following sections help illustrate why combi is important and why the NCMC was formed to bridge technical gaps:

- brief introduction to materials science,
- discussion and definition of polymers and their pervasiveness,
- review of traditional methods for materials research,
- introduction of combinatorial methods to materials science, and
- the rationale for NIST’s creation of the NCMC.

1.1 Overview of Polymers Science

Materials science is an interdisciplinary field that studies the structure, properties, and synthesis of materials (Smith, 2004). A “material” is broadly defined as any physical substance that is useful for human purposes, such as plastic or steel. Materials are often grouped into four principal categories:

- **Metals**: inorganic substances consisting primarily of metallic elements (e.g., gold, copper, and steel)
- **Ceramics**: inorganic substances consisting of metallic and nonmetallic elements (e.g., porcelain, glass, and rocks)

- **Semiconductors**: inorganic substances composed of metalloid elements (e.g., silicon and germanium)
- **Polymers**: typically organic (i.e., containing carbon atoms) substances composed of nonmetallic elements that form long molecular chains consisting of many repeating atomic units (from Latin, poly = many, mer = unit). Common synthetic polymers include plastics and rubber (Chung, 2007). Most naturally occurring materials like plant fibers are also polymers.

Materials are building blocks for products because of their properties—the way they respond to their environment. Copper's electrical property (conductivity) makes it a useful material for electrical wiring. Other important properties include mechanical (strength, elasticity), thermal (transmission of heat, heat capacity), chemical stability (corrosion), and optical properties (absorption, transmission, and scattering of light) (Bargolia, 2004).

Two factors govern the properties a material will exhibit: chemical composition and molecular structure. The importance of chemical composition in determining a material's properties is similar to the importance of ingredients in determining a cake's properties. If one bakes a cake with salt instead of sugar, its taste properties will be dramatically different (Chung, 2007).

However, even materials that have identical compositions can display different properties because of variations in how molecules are arranged or structured. A material's structure largely depends on how the material is created or its processing conditions. Both graphite and diamond are composed of pure carbon, yet they display different properties. Graphite is soft, while diamond is hard. These differences in properties are the result of differences in structure. The carbon atoms in graphite are organized in the form of sheets stacked on top of one another like a stack of paper. As a result, when force is applied to graphite, the sheets of carbon slip past each other. This is why it is easy to break the lead at the end of a pencil. In contrast, carbon atoms in diamond are bonded together in arrangements that resemble a pyramid that does not give as easily when force is applied (Chung, 2007).

The properties of a material are also affected by the structure of molecules in more subtle ways. In particular, when two chemicals are mixed together, the resulting mixture's properties will not only depend on the molecular structure of each individual chemical, but also on how the structures interact. One can intuitively understand the importance of how molecular structures interact by imagining each molecule as a toy block. The properties of a house built with these blocks, such as its appearance and stability, will not only depend on the shape of the individual blocks, but also on how they interact. A house made with square and rectangular blocks will have different properties than a house made with square and round blocks.

Molecular composition, structure, and structure at other length scales are important. For example, a material can be composed of the same molecules but be in an amorphous or crystalline state depending on the processing conditions of the material and temperature at end use. The molecules (molecular length scale) are the same, but the structure that arises from the intermolecular interactions (meso- or nano-length scale) determines if it is crystalline. The resulting differences in structure are reflected in the material's flexibility.

Among the largest output categories for the chemical industry, "polymers" is a term that refers to synthetic materials composed of carbon (organic) backbones. Polymers are molecules composed of carbon and other atoms covalently bonded together to form very long chains. Atomic repeat units are present that repeat themselves many times to form chains that can have molecular weights of 10,000 g/mol to 1,000,000 g/mol or more compared to small molecules like water (18 g/mol) or caffeine (194 g/mol). The molecular composition of a polymer, the number of repeat units (i.e., the molecular weight or how long the chain is), and the inter- and intramolecular interactions of the polymer chains determine the structure of the polymer. The structures, in turn, provide the polymer with its properties.

Polymers are commonplace; all plastics, paints, adhesives, coatings, rubber, and many other formulated products are polymeric. Table 1-1 lists 20 likely polymers that can be found in a typical office. Although the NCMC did not exclude siloxanes (silicon-containing materials) containing elements other than carbon, oxygen, and hydrogen, this report follows common usage and refers to organic polymers simply as polymers.

Table 1-1. Common Office Items Containing Synthetic Polymers

1. Writing pen (outer structure, rubber grip, container inside holding the ink, possibly polymers in the ink)
2. Computer (case work, circuit boards, packing of electronic components, adhesives, covering on all power and data lines, keyboard, mouse)
3. Phone (case work, electronics packaging, display screen, wire insulation)
4. Polyurethane coating desktop
5. Tape holder, the tape, and the adhesive on the tape
6. Carpet (threads, backing, adhesive attaching it to the floor)
7. Baseboard around the office
8. Office chair (foam padding, cloth covering, vinyl coverings)
9. Latex paint on the wall
10. Cover/diffuser on the room light
11. Light switch
12. All the insulation on the wires and data lines into the office
13. Wall and data sockets
14. Coatings on paper (e.g., shiny finish on wall calendar)
15. Plastic water bottle
16. Coating on coffee cup
17. Lunch bag, containers holding food in the lunch bag, guar gum as additive in food
18. Stain-resistant coating on clothing
19. Rubber soles on shoes
20. Coat made from nylon fabric

Consider poly(methyl methacrylate), or PMMA, commonly referred to as Plexiglas, which is renowned for its durability. Plexiglas's molecular composition and chain interaction make Plexiglas a substitute for glass that is strong, more flexible, and shatter resistant.

Polymers can be used in large solid forms, as thin coatings or films, or as additives to solutions to modify flow properties. Different polymers can be blended together. Additives to polymer blends, such as dyes or plasticizers, enhance polymer formulations. Fibers of polymer materials can be created: stronger and lighter materials than steel, such as for Kevlar fibers for bullet-proof vests; soft and pliable for a child's toy; thin and sticky for use as an adhesive; or thin, hard, and shiny for use as a protective coating on a piece of furniture.

The diversity of possible chemical compositions and combinations allows polymers to have a wide variety of properties for use in many applications. Yet, the large parameter space inherent with polymers (e.g., molecular composition, molecular weight, combination of components, processing conditions) also makes developing new polymer materials complex, expensive, and time consuming.

1.2 Traditional Methods of Polymers Research

The research activities involved with developing new polymer materials can be divided into two phases: **lead discovery** and **lead optimization**. Lead discovery is the identification of a material compound that is believed to possess desirable properties. The period during which that compound is further tested and improved before being released as a commercial product is referred to as lead optimization.

Until recently, lead discovery most often occurred by accident or through a slow trial-and-error process. Discovery by accident, though exciting and revolutionary at times, is unreliable, and duplication or reliable process development can be challenging as a consequence. For instance, the discovery of Teflon by Roy Plunkett of DuPont occurred by accident while he was attempting to develop a new refrigerant compound. Plunkett's new material exhibited extraordinary properties, including high melting temperature, resistance to chemicals, and low surface adhesion, making it excellent for a wide variety of applications such as making cookware. But it took DuPont researchers 3 years to develop a reliable process for manufacturing it (Strauss, 2002).

More deliberate methods of materials discovery follow a cycle of designing, making, testing, optimizing, and analyzing candidate compounds. As an example of this materials discovery process, consider the development of a new plastic material with improved strength and heat resistance for making engine parts. Researchers would first consider existing materials that come close to meeting the requirements and improvements to them. If researchers concluded that they needed to develop a new material, like a new polymer or combination of existing materials, they would then design experiments. Samples would be individually prepared and tested for the properties of interest, such as softening temperature, strength, and hardness.

After these tests are complete, researchers analyze output data to determine whether any of the samples meet the performance criteria. If the sample displays the desired characteristics, it becomes a “lead.” If the substance does not meet the criteria, the researcher returns to the beginning of the cycle and iterates this process. Once a lead is discovered, it enters the optimization phase to determine whether the material can be improved upon to exhibit the desired property or properties more strongly. This phase may include mixing the material with other materials or improving on the production process used to create the material itself.

Traditionally, all of these activities were performed manually. Teams of scientists were required to select and synthesize sample materials, test them for desirable properties, and then attempt to optimize those properties. Given that lead discovery and optimization often involve hundreds of samples and several tests per sample, materials R&D can be an expensive and slow process. The R&D for bringing a new product to market can take 2 to 10 years and cost in excess of $20 million (De Lue, 2001).

In a 1970 publication, Dr. Joseph Hanak, then an industrial chemist at RCA Laboratories and an early thought leader in combi for materials science, was frustrated by the slow process of materials research: “[the current] approach to the search for new materials suffers from a chronic ailment, that of handling one sample at a time in the processes of synthesis, chemical analysis and testing of properties. It is an expensive and time consuming approach, which prevents highly trained personnel from taking full advantage of their talents and keeps the tempo of discovery of new materials at a low level” (Hanak, 1970).

1.3 Introduction of Combinatorial Methods to Polymers Science

The slow and inefficient character of materials research in which samples were individually manually prepared was the driving force behind developing combi for polymers. Scientists began to envision processes where many different samples with different compositions could be made at one time. Combi offered materials scientists an alternative to traditional research techniques because they enable the creation of a large number of related chemical samples (known as **libraries**) and the rapid analysis of the properties [known as “**high-throughput screening**” or “**high-throughput experimentation (HTE)**”].

Combi was first successfully used in the pharmaceutical industry in the early 1990s as a means to increase the speed of drug discovery and, therefore, lower the cost of bringing new drugs to market (PhRMA, 2007). In combinatorial chemistry, a large number of related chemical compounds are made through automated synthesis and are then screened quickly using simple tests for appropriate activity. For example, does compound A react or not react with enzyme B as indicated by a color change?

An early illustration of the potential benefit of applying combi came in 1995 when researchers at Pfizer declared that the drug company had a compound in clinical trials that would not have been discovered without combinatorial methods (Thayer, 1995). According to the company’s research staff, the breakthrough did not arrive until they had synthesized nearly 900 variations of the compound, a number they would never have achieved using manual methods.

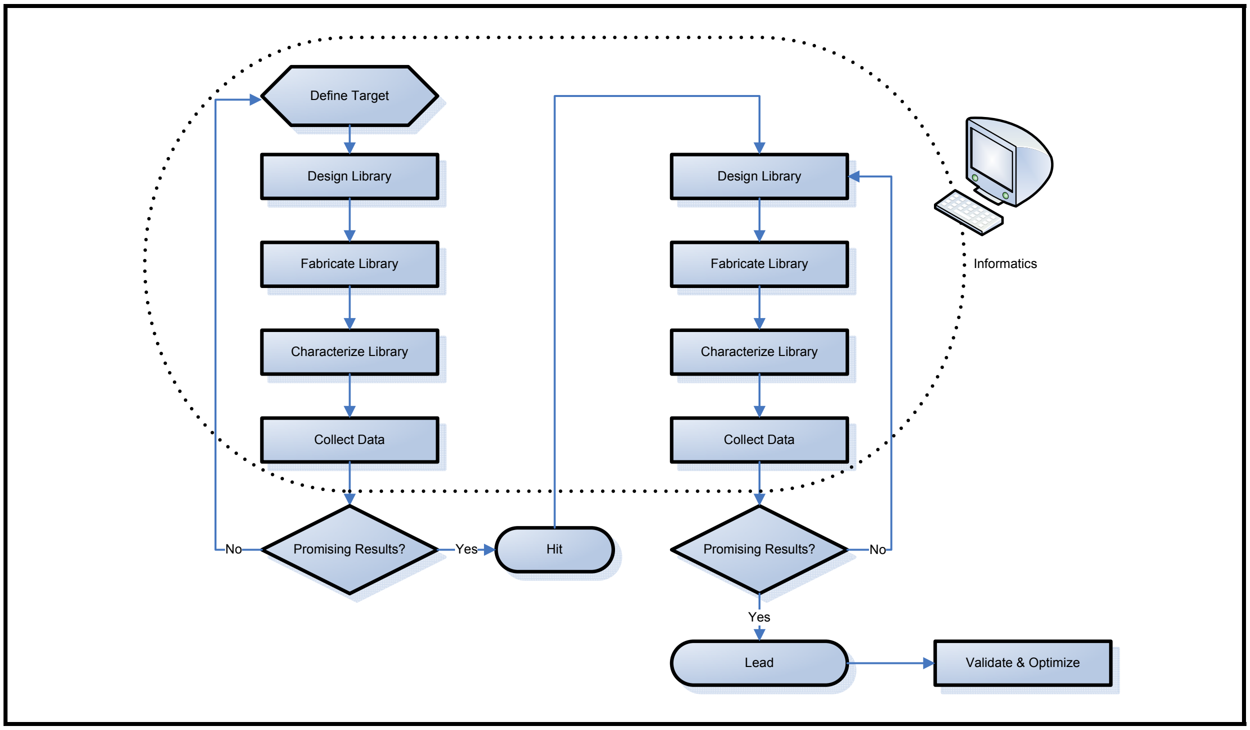
Inspired by the success of combi in pharmaceutical research, in the late 1990s, researchers began to seek avenues for applying the combinatorial and HTE philosophy to materials science. Foremost among the challenges they faced was fundamental: when combinatorial techniques are applied to drug research, screening compounds can be fairly straightforward and based on yes-or-no results. The range and diversity of properties, along with the range of factors affecting them, make combi for materials science far more difficult than with “classical” combinatorial chemistry.

1.3.1 Key Concepts in Combi

Combi can be applied to improving each stage of the experimentation cycle described in Section 1.3 to create a seamless “**combinatorial workflow**.” This workflow comprises four steps, all of which are integrated using an informatics system (Figure 1-1).

Researchers begin by using their existing knowledge of materials science to design an experiment to identify material exhibiting properties X and Z. This involves identifying materials that are likely to exhibit the properties of interest and then determining how these materials

Figure 1-1. Combinatorial Workflow Cycle
A robust combinatorial system for materials research includes an informatics system to handle data and guides the research process.



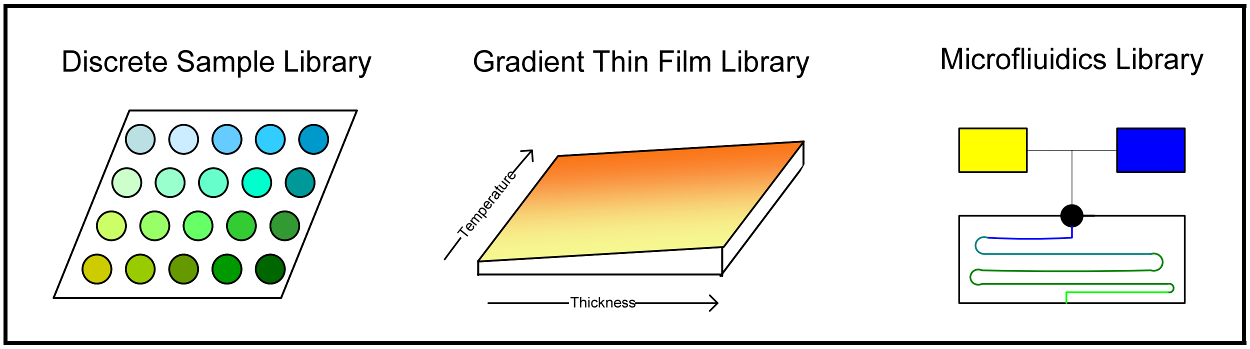
should be synthesized, how they should be tested, and finally how the results of the tests will be analyzed.

Library fabrication is typically automated using robotic systems that are coordinated by the informatics system. The design and fabrication of this library typically depends on the experiment being conducted. Two examples of libraries used in polymer science are **discrete libraries** and **continuous gradient libraries**. Discrete libraries have tiny amounts of material samples arranged into individual wells or arrays of miniature specimens. Each well may contain a different material sample that will be subjected to the same test or each well may contain the same type of material sample that will be subjected to different tests in each well. Examples of continuous gradient libraries include continuous films of material spread onto a plate where properties such as a temperature, thickness, or composition are varied along each axis. **Microfluidics libraries** permit researchers to analyze variations in polymer formulations over a variety of processing conditions or compositions. An illustration of each type of library is provided in Figure 1-2.

After sample libraries have been fabricated, the samples are analyzed with automated systems that rapidly test each sample in the library for the desired properties. The test in question typically depends on the property being analyzed. For example, peel-off tests might be used to determine the adhesion properties of material in the library if researchers are interested in identifying a material of a specific stickiness.

Figure 1-2. Discrete Sample, Continuous Gradient Thin Film, and Microfluidics Libraries

A computer-controlled system deposits samples of varying composition into individual wells arranged in a matrix to form a discrete library of samples. A flow coating technique is used to make a polymer film that varies in thickness in one direction and a temperature gradient stage is used to vary temperature in another direction, thus creating a whole range of conditions in a single sample. A microfluidics system creates variations in formulation in a reactor.



The informatics system records the test results for each chemical compound that researchers then use the informatics system to analyze these results. If the experiment in question is being conducted to discover a new material, these results will help researchers determine whether particular material samples are leads. If the experiment is being conducted as part of the lead optimization process, these results will help researchers determine how they can strengthen the properties exhibited by the lead materials.

Analytical results can also be used to inform subsequent experiments because they may help researchers better understand what materials (or combination of materials) exhibit which properties. As a result of this feedback into experiment design, the combinatorial workflow takes on a circular flow quality that is meant to foster improvements in future experiments while giving faster results across a broader parameter space today. This combinatorial workflow aims to significantly lower cost and time per lead in developing a new product.

1.3.2 Technical Challenges to Applying Combi in Polymers Research

Screening a fabricated library rarely presents researchers with a simple yes/no answer. Because typically more than one property is of interest, and because material properties are a continuum of values (versus reacts or does not react), the set of desired properties may be physically or chemically incompatible. Materials scientists must make trade-offs between properties such as hard (high modulus) yet brittle (low strength) versus soft but elastic. Combi and materials science in industry is a continuum starting with discovery, transitioning to optimization, and ending with a product.

Whereas in combinatorial chemistry in the drug industry, molecular composition of a one-component system is the standard focus, the focus in materials development is on multicomponent systems. Formulation is standard; more than one type of polymer may be mixed together in combination with additives to obtain the desired combination of properties. Furthermore, materials scientists face the challenge of working with material that is typically viscous and is processed with solvents or at temperatures that would damage or destroy the equipment pharmaceutical companies use for their combi workflows.

The three interrelated challenges of materials discovery—that materials are tailored for specific applications, materials are formulated from many components, and each component has a structure and intricate behavior—are the root of the challenge of using combinatorial approaches for materials. In recent years, property specifications for materials mandated by end users have simultaneously increased and become more complex (Wicks and Bach, 2002). This increasing difficulty in developing coatings formulations led Douglas Wicks and Hermann Bach of the Bayer Corporation (a current NCMC member organization) to declare that a “revolution” was needed in coatings science (Wicks and Bach, 2002). In a paper presented at the Water-Borne & Higher Solids and Powder Coatings Symposium, Wicks and Bach argued that this “revolution” would be provided in the form of combinatorial methods.

A small number of firms emerged to produce and market combinatorial workflows for HTE for discrete sample libraries, offering solutions based on robotics and automaton. But these providers were not fully addressing key challenges for thin films and microfluidics libraries, including

- library design across multivariate parameter spaces;
- library fabrication, including materials handling, production, mixing, deposition, and variation of processing conditions;
- high-throughput measurement methods and metrics;
- data capture, analysis, and management tools; and
- informatics for instrument automation, data mining, analysis, and visualization (Hewes, 2000).

1.4 NIST's Entry into Combi: Addressing Technical and Market Barriers

Despite the promise combi held for materials discovery and the downstream products enabled by new materials, technical barriers obstructed combi's practical introduction. The equipment, measurement infrastructure, and analytical tools were inadequate. Indeed, systems capable of fabricating gradient and microfluidics laboratories for organic polymers were nonexistent. The concepts and philosophy were present, but the technology infrastructure, culture, and perception that combi could be applied to polymers were not. Compounding the problem was a lack of high-throughput measurement systems to acquire data rapidly from libraries that were more than a simple yes-no solution space.

It is unknown to what extent private-sector organizations successfully implemented combi in their R&D and process engineering programs in advance of the NCMC, but those that did likely incurred high costs. It is doubtful that they would have disclosed their efforts beyond exchanges with contract engineering and equipment vendors. (Research groups in academia, such as the Center for Nanoscale Science and Engineering at North Dakota State University, were in the early stages of launching programs using combi for discrete libraries when NCMC launched in 2002.)

Building a high-throughput workflow based on robotics is capital intensive, requiring start-up investments ranging between $8 and $20 million (Symyx, 1999). An Advanced Technology Program (ATP) white paper published in 2000 with the assistance of public- and private-sector researchers argued that "discontinuous innovation in generic and/or modular hardware and software technologies will be necessary to drive down costs and facilitate its implementation in industrial sectors that have lower returns on R&D investment, such as exist in the chemical and materials industries" (Hewes, 2000).

NIST's involvement in combi initially took the form of a research project undertaken by NIST researchers Eric Amis, Alamigir Karim, and Carson Meredith that developed gradient thin films libraries. The results of NIST's research were first presented in 1999 at the Gordon Conference on Reactive Polymers, Ion Exchange, and Adsorbents (Meredith et al., 1999) and were ultimately published in a series of papers in 2000 (Meredith et al., 2000; Meredith, Karim, and Amis, 2000). This initial research was leveraged to garner NIST funding (2001) in order to build a modest program in combinatorial methods for polymer thin films.

The enthusiastic response with which the thin films research was met, ATP's white paper series identifying technical challenges, and comments NIST received from stakeholders suggested that NIST could serve a role. The combi community was fractured; there was no independent coordinating body to advance combi's science and raise its profile as a more effective and alternative research paradigm for advanced materials. NIST conducted an assessment and solicited comments via conference circuits cosponsored by the Knowledge Foundation, which permitted NIST scientists to further gauge interest, identify needs, and strategize a role for the emerging NIST effort.

The potential impact of developing effective equipment and techniques in combinatorial polymers materials research and the sizable challenge to developing workflows for materials research led the NIST Polymers Division to develop the NCMC program. Following a brief planning period, NIST launched the NCMC in early 2002 to provide a leadership role by sponsoring and coordinating an "open-source," precompetitive forum to accelerate combi in polymers.

1.5 Report Organization

This report is organized as follows:

- Chapter 2 presents an overview of the NCMC with an emphasis on the use of the consortium approach.
- Chapter 3 reviews the Center's technical contributions.
- Chapter 4 discusses how combi impacts the R&D activities of the key industries where it is being used or has potential to be used in the future.
- Chapter 5 presents the methodology for conceptualizing economic impacts and quantifying economic benefits.
- Chapter 6 presents the analytical results from economic modeling.
- Chapter 7 concludes with remarks about the broader implications of the NCMC's impacts and the effectiveness of NIST's use of a consortium approach as the research program model.

2. OVERVIEW OF THE NIST COMBINATORIAL METHODS CENTER

The NCMC's mission is to promote industrial adaptation of combinatorial and high-throughput measurement methods that serve to accelerate the discovery, development, and optimization of innovative materials products. The Center furthers its mission by building the technology infrastructure supporting combi, partnering with industry on research priorities, transferring technology to the public domain, and lending thought leadership to the research community. This chapter explores the NCMC's consortium approach, operational structure, and nontechnology outputs. Details on NCMC's technology contributions are discussed in Chapter 3.

2.1 NCMC's Consortium Approach

Three overarching objectives characterized the NCMC when it was launched in January 2002:

- Provide technology to overcome technical barriers to combinatorial and high-throughput experimentation for organic polymers.
- Disseminate research findings rapidly, offer instruction and best practices, and proactively engage the materials science community to raise awareness of the advantages of combinatorial and high-throughput experimentation for materials discovery.
- Establish a forum wherein NIST, industry, and academics could exchange ideas and techniques, identify technology needs, and set research needs.

At the time of the NCMC's creation, NIST Polymer Division's leadership and leading academics believed that the existing knowledge base for combi was locked within silos at major corporate R&D centers and technology vendors. The commercial infrastructure for HTE using discrete sample libraries was more established, particularly through the efforts of Symyx and other automated systems vendors. The absence of any precompetitive forum for discussing combi inhibited even the discussion of general topics.[1] Comments received following NIST's solicitations at Knowledge Foundation meetings suggested that an open model where industry and academia could drive the research agenda and share equally in all knowledge gains, with no time advantage, would be most effective.

The NCMC adopted a consortium model to maximize technology transfer from the NCMC to industry and academia. The Center would offer novel technology solutions that minimized costs and maximized throughput. NIST aspired to feed research by academic and industrial researchers by releasing tools, data, and methods as they are developed. Thus, the NCMC was conceived as an "open-source" community supported by NIST and industry members' annual fees. The NCMC would develop infratechnology in response to stated needs and disseminate

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[1] Precompetitive forums offer researchers at competing organizations the opportunity to discuss and jointly address or collaborate on issues arising during the early stages of a technology's development and adoption.

them through workshops, papers, and presentations. A condition of membership is that any technology developed within the Center would be published and freely available. All NCMC innovations enter the public domain. The NCMC would also be a nucleus that would coordinate and drive symposia and national and international meetings and interface with the American Chemistry Society (ACS) and the Materials Research Society (MRS), the leading professional associations for materials science.

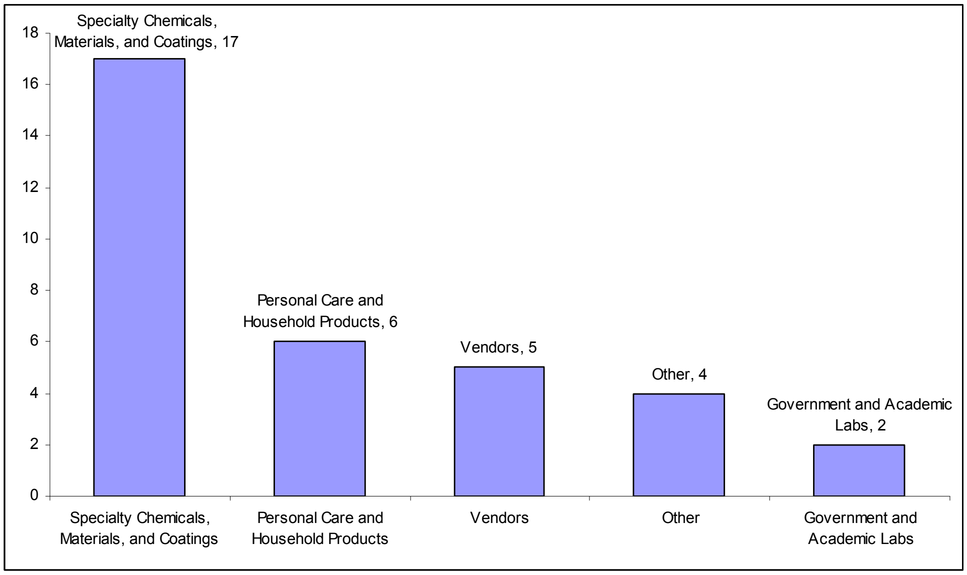
2.2 NCMC Structure

The NCMC has a two-tier membership structure built on a foundation of NIST expertise in materials science and chemical engineering. Given that the Center focuses on combi for polymers, most members are specialty chemicals, coatings, or advanced materials companies (see Figure 2-1). However, the NCMC leadership partners with and invites to NCMC meetings industrial and academic researchers in other materials domains given that the development and application of combi and high-throughput experimentation are priorities for materials research in general, not just polymers.

2.2.1 NCMC Staff and Operations

The NCMC is staffed with a core research and administrative staff of NIST employees from the Polymers Division. In addition, researchers from other NIST units lend their expertise to NCMC projects and activities as needed. The NCMC is not the only group at NIST engaged in research into combi methods or applying combi. NIST's ceramics and semiconductor research groups

Figure 2-1. NCMC Members and Alumni, by Industry



Source: NIST Combinatorial Methods Center are also developing and using high-throughput experiments in their work. Thus, there is an element of cross fertilization (economies of scope) among the several materials domains.

The majority of NCMC's full-time staff are postdoctoral researchers ("postdocs"). Since 2002, more than 25 postdocs have left the Center following their 2-year positions to join universities and corporate research divisions, many of which were NCMC members. The benefits of this approach are that the NCMC regularly draws fresh talent and routinely graduates talented researchers with hands-on training and a diversified skill set in these new and exciting techniques.

NIST staff and NCMC postdocs are complemented by hosted researchers from universities, member companies, and national research laboratories. Hosting researchers is a key component of the education pillar of NCMC's mission and vital to the direct transfer of technology to the private sector.

2.2.2 General Membership

Two NCMC membership levels are available for industry: general membership and focus project participation. Members at the nonproprietary level pay approximately $10,000 per year to participate in the NCMC. This membership includes

- participation in semiannual meetings organized in response to stated needs or emerging issues in high-throughput experimentation (see Table 2-1);
- access to electronic resources through the NCMC Web site, including guides, protocols, strategies, and measurement techniques;
- access to workshops, demonstrations, and prepublication technical papers; and
- on-site demonstrations of new techniques and apparatus for HTE.

Organizations that are not members of the NCMC have access to the consortium's accomplishments through workshops, journals, and conferences, but they do not have access to them on a prepublication basis. Thus, they incur the lag between writing papers, acceptance, and publication.

Current and former NCMC members characterized the benefit of membership in terms of impacts within their organization and not in terms of the activities of membership. In the words of one former member: "One of the advantages of working with NIST is [that] you're working with a group of very smart people [who] are far more advanced in terms of where you are on the [combi] learning curve." Many members joined the consortium as part of their program for implementing HTE. Common benefits cited by members include

- demonstration of what was possible with combi;
- inspiration for new research approaches and the creation of new methodologies;

Table 2-1. NCMC Semiannual Meetings: Topics and Private-Sector Attendance Counts

Meeting	Topic	Year	Industry Attendees
NCMC-1	Library Design and Calibration	2002	16
NCMC-2	Adhesion and Mechanical Properties	2002	42
NCMC-3	Combinatorial Informatics	2003	24
NCMC-4	Polymer Formulations	2003	54
NCMC-5	Combinatorial Processing & Characterization	2004	37
NCMC-6	Advanced Materials Forum	2004	27
NCMC-7	Adhesion and Mechanical Properties II	2005	24
NCMC-8	Polymer Formulations II	2005	24
NCMC-9	Combinatorial Methods for Nanostructured Materials	2006	29
NCMC-10	Completing the Combi Loop: Examining Persistent Challenges in Implementing Combinatorial Materials Science	2006	26
NCMC-11	Complex Interfaces: Library Design & Performance Measures	2007	32
NCMC-12	Data Acquisition, Management, and Handling	2007	20
NCMC-13	Advances in Library Fabrication	2008	14
NCMC-14	DOE-EERE/NIST Joint Workshop on Combinatorial Materials Science for Applications in Energy	2008	8

Source: NIST Combinatorial Methods Center.

- validation of research strategies and invalidation of others that, if pursued, would likely have failed;
- accelerated combi adoption and scale-up; and
- knowledge benefits of working with researchers with similar interests but different perspectives because of different materials domains.

Annual NCMC membership fluctuated and largely corresponded with the research community's interest in combi in general as well as the interest in topics the NCMC was exploring at any given time. Table 2-2 presents a chronology of NCMC membership by company. Membership was lowest in 2002 and 2003, which was a period when many companies became "disillusioned" with combi because of persistent challenges integrating combi into their workflow. Membership peaked in 2004 with 23 members and, in subsequent years, was around 15 companies per year. Specialty chemical and materials companies Air Products, Atofina, BASF, Bayer Materials, and National Starch have been members in each year of the NCMC's existence.

2.2.3 Focus Projects

NCMC focus projects offer members the additional opportunity to sponsor and collaborate with NCMC staff on projects aligned with their particular research interests and needs. The benefits of focus project participation are threefold; members' participation enables them to

Table 2-2. Chronology of NCMC Membership

Company	2002	2003	2004	2005	2006	2007	2008
3M Company	■	■					
Accelrys Inc.		■	■				
Air Force Research Laboratory	■	■	■	■			
Air Products and Chemicals, Inc.	■	■	■	■	■	■	■
Akzo Nobel N.V.	■	■	■				
Arkema Inc. (formerly Atofina)			■	■	■	■	■
ATRP Solutions						■	■
Avon Products, Inc.					■		
BASF SE	■	■	■	■	■	■	■
Bayer AG	■	■	■	■	■	■	■
Boston Scientific				■	■		
BP PLC			■	■			
Chemistry Innovation						■	■
Dow Chemical Company		■	■	■	■	■	
Eastman Chemical Company			■	■			
Exxon Mobil Corporation	■	■	■	■	■	■	
Gillette (now part of Procter & Gamble)	■						
Honeywell International, Inc.	■	■	■	■	■		
Hysitron, Inc.			■	■	■	■	
ICI/National Starch & Chemicals	■	■	■	■	■	■	■
Insight Faraday					■		
Intel Corp			■	■	■		
L'Oréal SA				■	■	■	■
LORD						■	
Michelin		■	■				
PPG Industries, Inc.		■	■	■	■		
Procter & Gamble Co.	■	■	■	■	■		
Rhodia	■	■	■	■	■	■	
Rohm and Hass Co.	■						
Sealed Air Corp.			■				
Symyx Technologies, Inc.		■	■		■	■	■
Unilever PLC					■	■	■
University of Southern Mississippi			■	■	■	■	
Vecco Instruments Inc.			■	■	■		
Vistakon						■	■

Source: NIST Combinatorial Methods Center.

- help guide and scope focus projects;
- gain direct, ongoing knowledge in the project area; and
- acquire information and insights in "real time" as opposed to waiting for NCMC semiannual meetings or publications.

The advantage members gain through participation in focus projects is simply that their researchers acquire the expertise and tacit knowledge benefits of NCMC postdocs and staff involved in the project as they were executing it. They are then able to transfer the technology in real time to their home research labs. As with general membership, there is no cooperative research and development agreement (CRADA), and all knowledge and technology developed as part of the focus project are nonproprietary and fully publishable.

The NCMC members' time advantage over competitors can be illustrated this way: if a focus project lasted 2 years, and it took an additional 6 to 9 months to have a paper accepted for publication, and 3 to 6 months before the article appeared, then member companies have a multiyear time advantage in addition to the tacit knowledge experience over their nonmember competitors.

Although costs vary by project, on average, members pay approximately $70,000 to participate in focus projects in addition to their annual membership fee and labor and travel expenses for their employees. Focus projects last 2 to 3 years, and the annual participation fee is usually $20,000 to $30,000. NCMC's four focus projects included

- High-Throughput Interfacial Tension Measurements,
- High-Throughput Methods for the Evaluation of Adhesive Properties,
- High-Throughput Flammability Test Methods for Compositionally Graded Samples, and
- High-Throughput Modulus Measurements of Hydrated Polymer Gels.

2.3 Nontechnology Outputs

In the views of interviewees, equally as important to NCMC's technical accomplishments are the Center's contributions to the development of human capital and a technical community focused on combi. Human capital development consisted largely of NCMC postdocs who offered industry and academia talented, multidisciplinary researchers and hosted researchers from NCMC member organizations and international research groups. A significant proportion of the Center's mission was focused on outreach, and the NCMC organized and led symposia at MRS and ACS meetings, among others, that demonstrated the possibilities with combi to large numbers of researchers.

2.3.1 Human Capital Development: Postdoctoral and Hosted Researchers

Many research groups are in the early years of adopting combi and HTE, and the NCMC postdocs are a talent pool that offers expertise as groups adopt combi workflows. More than 25 researchers have completed postdocs with the NCMC and are working in academia, private industry, and government. Most postdocs bring their employers connections, hands-on knowledge, and research program management skills beyond those of newly minted PhDs. The additional value NCMC postdocs offer is hands-on experience developing new approaches in an industry-focused, dynamic research environment. Several NCMC postdocs were hired explicitly because they had the broad experience from their NIST years as well as a deep understanding of the issues and challenges in moving to a high or high*er*-throughput research environment. The comparable amount of time for training a non-NCMC postdoc to reach the same knowledge and technical sophistication level was estimated by their employers to be 8 months to a year.

2.3.2 Conference and Symposium Sponsorship

Interviewees' remarks suggest that demonstrating what was possible with combi was equally as important as the actual methods and tools. The NCMC engaged nonmembers through two primary mechanisms: technical papers and conference proceedings, and organization and sponsorship of conferences and symposia.

Organizing tracks and symposia at major MRS and ACS conferences as well as at more targeted audiences for Knowledge Foundation and Gordon Conference meetings offered the staff access to audiences outside of the immediate membership (see Table 2-3). Indeed, the NIST staff and their projects were central to starting the Gordon Conference series on combi. Certainly the staff maintain professional relationships with other researchers, but organizing symposia offered the Center the opportunity to present formally and provide evidence of the consortium's technical accomplishments.

Many attendees with whom we spoke did not adopt the technology as presented; their principal take-away point was that the Center demonstrated what was possible with combi and that combi could be applied efficiently to polymers without necessarily investing in costly automated workflow systems. Yet, there are also cases where NIST's validation of combi aided in companies deciding the capital investment was worth the investment to achieve their particular goals.

2.3.3 Papers and Proceedings

Technical papers published in the peer-reviewed literature facilitated the transfer of knowledge generated by the NCMC into the public domain for use by the entire materials science community. RTI performed a brief citation analysis for all 146 papers published by NCMC staff between 2000 and December 2007 which collectively received nearly 1,400 citations (as of January, 2009). Table 2-4 lists five of the most frequently cited papers published.

The paper that generated the most citations was written by Christopher Stafford and colleagues on buckling-based metrology for measuring the elastic moduli of polymeric thin films (Stafford et al., 2004). This paper generated 123 citations as of February 2009. The next three most-cited papers—Meredith et al. (2000), Meredith, Karim, and Amis (2000), and Ragavan et al. (2000c)—addressed the fabrication and use of continuous polymer libraries. These early NCMC papers received a combined total of 295 citations by researchers at a variety of universities as

Table 2-3. NCMC-Sponsored or -Organized Symposia at Major Scientific Meetings

Meeting
1. 5th International Conference on Combinatorial and High-Throughput Materials Science, Kloster Seeon, Germany, October 2008
2. Combinatorial and Informatics Methods in Materials Science IV, Boston, MA,
3. Combinatorial and High-Throughput Polymer Chemistry, Chicago II, ACS Spring Meeting 2007, March 2007
4. 4th International Workshop on Combinatorial Materials Science and Technology, San Juan, Puerto Rico, December 2006
5. Combinatorial and Informatics Methods in Materials Science III, Boston MA, MRS Fall Meeting 2005 (Published Proceedings)
6. Combinatorial Approaches to Materials II, Washington DC, ACS Fall Meeting 2005
7. APS March Meeting 2005, Los Angeles CA, Parallel and High-Throughput Experimentation for the Physical Sciences
8. Combinatorial Approaches to Materials, Anaheim CA, ACS 2004 Spring Meeting
9. Combinatorial Methods in Adhesion, Wilmington, NC, Adhesion Society 2004
10. 3rd International Workshop on Combinatorial Materials Science and Technology, Okinawa, Japan, December 2004
11. Knowledge Foundation COMBI 2004: 6th Annual International Symposium on Combinatorial Approaches for New Materials Discovery, Arlington, VA
12. Combinatorial and Artificial Intelligence Methods in Materials Science II, Boston, MA, MRS Fall Meeting 2003 (Published Proceedings)
13. Knowledge Foundation COMBI 2003: 5th Annual International Symposium on Combinatorial Approaches for New Materials Discovery, San Jose, CA
14. New Gordon Conference: Combinatorial and High Throughput Materials Science, New Hampshire, 2002
15. Knowledge Foundation COMBI 2002: 4th Annual International Symposium on Combinatorial Approaches for New Materials Discovery, San Diego, CA
16. Combinatorial and Artificial Intelligence Methods in Materials Science I, Boston, MA, MRS Fall Meeting 2001 (Published Proceedings)

Source: NIST Combinatorial Methods Center

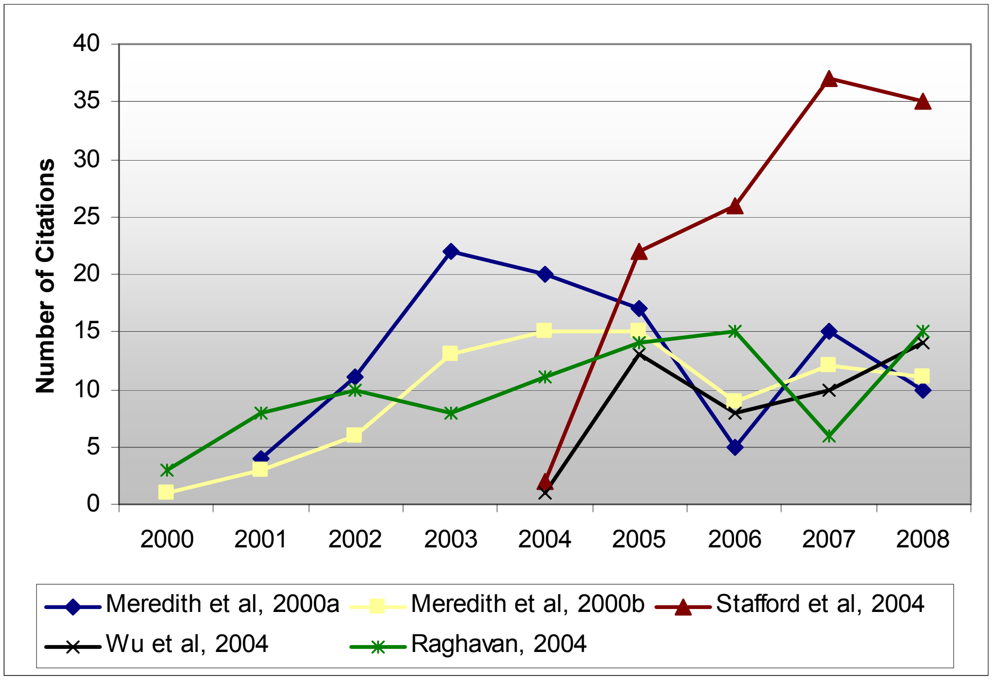
Table 2-4. List of Five NCMC Papers Most Frequently Cited in the Literature

Publication Information	Number of Citations
Stafford, C.M., C. Harrison, K.L. Beers, et al. 2004. "A Buckling-Based Metrology for Measuring the Elastic Moduli of Polymeric Thin Films." *Nature Materials* 3(8):545-550.	123
Meredith, J.C., A.P. Smith, A. Karim, et al. 2000a. "Combinatorial Materials Science for Polymer Thin-Film Dewetting." *Macromolecules* 33(26):9747-9756.	104
Raghavan D, Gu X, Nguyen T, et al. 2000. "Mapping Polymer Heterogeneity Using Atomic Force Microscopy Phase Imaging and Nanoscale Indentation." *Macromolecules* 33(7):2573-2583.	91
Meredith, J.C., A. Karim, and E.J. Amis. 2000. "High-Throughput Measurement of Polymer Blend Phase Behavior." *Macromolecules* 33(16):5760-5762.	85
Wu, T., Y. Mei, J.T. Cabral, et al. 2004. "A New Synthetic Method for Controlled Polymerization using a Microfluidic System." *Journal of the American Chemical Society* 126(32):9880-9881.	47

Note: Citation counts obtained through Web of Science academic database, February, 2009.

well as private institutions such as GE, BASF, Bayer, and Procter & Gamble. Another frequently cited paper (48 citations) focused on microfluidics for polymers in organic solvents (Wu et al., 2004). The number of times each paper was cited each year is illustrated in Figure 2-1.

Figure 2-1. Yearly Citation Analysis for Major NCMC Publications



3. NCMC TECHNICAL ACCOMPLISHMENTS

The NCMC made significant contributions to the fabrication and testing of combi polymer libraries, validating the application of combi methods to polymer materials research and stimulating U.S. industry to adopt combi and think innovatively about applying the concept of combi to polymers research. Using combi, researchers are able to rapidly map out structure–property relationships in systems with multiple parameters. This enables developers to more rapidly and efficiently develop new materials, optimize a material for a particular application, and respond to changes in raw materials and the market. Additional benefits may include reduction in materials consumed and waste generated while developing a new polymer material because of reduced sample size and development of more robust materials because of the ability to test over a much broader range of conditions or explore a larger combination of components.

NCMC's work touched on each phase of the combi workflow and three different platforms for library creation (see Table 3-1): gradient thin films, discrete libraries created by robotic dispensing systems, and microfluidics. Testing of polymer libraries frequently requires new or modified equipment to speed up the measurement process creatively. As summarized in Table 3-2, NCMC innovated more than six measurement methods and made contributions to several more for library measurement. By design, combi generates large volumes of data that have to be captured, processed, and reported in a meaningful manner. This informatics aspect of combi was also a research area for the NCMC. The discussion in this section is organized by library type.

3.1 Combi Using Continuous Gradient Approaches for Thin Polymer Films

The most mature and frequently cited research in the academic literature is NCMC's gradient thin-film technology. The basic concept of creating and using gradients is NCMC's most broad-reaching technical contribution. NCMC developed methods to create gradients in thickness, temperature, surface energy (e.g., water repellency), and composition.

An example helps illustrate the gradient thin-film concept and the ingenuity of NCMC staff. Consider that a new coating is being developed that requires the blending of two different polymers: polystyrene (PS) and polyvinylmethylether (PVME). One problem with blending polymers is that they may phase separate. That is, rather than having one nice film with both polymers mixed intimately together, a cloudy film is formed that has domains rich in PS and domains rich in PVME. Imagine a hypothetical situation in which oil and water mix together at high temperature into one clear solution (or phase), but upon cooling the oil and water separate (phase separate), forming a cloudy solution. In our polymer thin-film example, phase separation is a function of composition and annealing temperature, and the variations in the library can be used to assess variations in composition or processing temperature.

Table 3-1. NCMC Platforms for Library Creation

Platform and Library Properties	NIST Original
Gradient thin film libraries for polymers	
Thickness gradient	Yes
Surface energy gradient (UV ozone)	Yes
Temperature gradient	Yes
Composition gradient	Yes
Graded chemically patterned substrates	Yes
Discrete sample libraries	
Composition gradients for solutions	
Composition gradients for films and “dots” (blobs of polymer)	
Temperature gradient in position or time	
Microfluidics libraries	
Composition gradients, discrete library by droplet	
Composition gradients with reaction in organics, discrete library by droplet	Yes
Solution-deposited films (brushes) with chemical/composition gradient, continuous sample (film)	Yes
Solution-deposited copolymer films with chemical/thickness gradient, continuous sample (film)	Yes

Traditionally, a researcher would prepare individual samples, each with varying amounts of PS and PVME in them and then vary the temperature of each sample. Instead of this slow process of individual samples, a continuous sample that varies in composition in one direction and temperature in another can be made. This is a continuous gradient sample library. Figure 3-1 shows such a gradient sample where polymer PS content is varied along the x-axis and annealing temperature along the y-axis (Meredith, Karim, and Amis, 2002).

Figure 3-1. Gradient Thin-Film Sample
A polymer thin film with a gradient composition of polystyrene and polyvinylmethylether in the x-axis and temperature gradient in the y-axis provides a library of samples that took 2 days to make instead of weeks. The phase separation boundary of PS and PVME is clearly seen. White circles are traditionally collected data indicating the phase boundary (Meredith, Karim, and Amis, 2002).

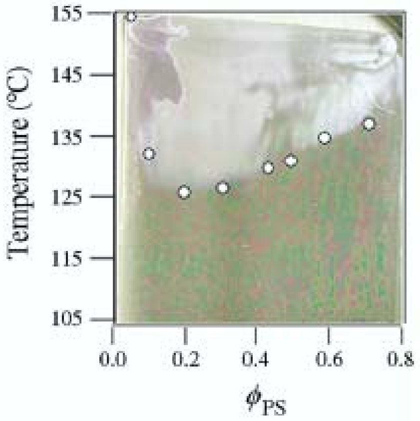


Table 3-2. Materials Property Measurement for NCMC Library Platforms

		Type of Library					
Material Property	**Measurement**	**Continuous Thin Film**	**Discrete Thin Film (sectioned)**	**Microfluidics Discrete Droplets**	**Continuous Fluidics Sample**	**Discrete Samples via Other Process**	**NIST Original**
Adhesion	Multilense contact (MCAT)	●	●				Yes
Adhesion of PSA	Adhesive peel test	●	●				
Adhesion-bonding	Edge delamination test		●			●	Yes
Chemical composition	Ion mass spectroscopy, TOF-SIMS	●	●			●	
Composition, rxn conversion	FTIR	●	●	●	●	●	
Composition, rxn conversion	Raman spectroscopy			●		●	
Craze resistance	HT craze testing on copper grids	●					Yes
Interfacial tension	Fluidics interfacial tension device			●			Yes
Modulus	Film buckling (SIEBIMM)	●					Yes
Modulus, soft films	Reverse buckling (reverse SIEBIMM)	●					Yes
Morphology	Automated AFM/SPM	●	●				
Morphology	Near field polorimetry	●	●	●	●	●	
Morphology	Light scattering; DLS, SALS			●		●	Yes
Morphology	SANS/SAX					●	
Morphology	Electron Microscopy	●	●			●	Yes
Morphology	Automated microscopy	●	●	●	●	●	
Surface energy	Automated contact angle measurement	●	●			●	
Translation rate	Automated microscopy						
Thickness	FTIR					●	
Thickness	Interferometery	●	●			●	
Thickness	AFM	●	●				
Thickness	Elipsometry	●	●				
Viscosity	Fluidics viscometer				●		Yes
Viscosity/rheology	Multisample rheometer					●	Yes

Once the library is fabricated it is ready for measurement. In the above example, the phase behavior is directly observable by viewing the clouding of the polymer film at conditions where phase separation occurs. Part of the ingenuity of gradient libraries is that they can be self-**reporting**. In other words, the solution space is directly observable. Measurement can include color change and light scattering. The boundary between conditions providing for one phase or two is clearly seen in Figure 3-1. The white circles are data points from traditional samples and light-scattering measurements overlaid on the coordinate system created by the gradient sample (PS content x-axis and temperature y-axis). NCMC's novel approach of preparing this gradient sample reduced preparation and measurement from weeks to just 2 days. NCMC's successes with gradients stimulated a number of industrial and academic researchers to develop gradient methods for their own applications.

NCMC also developed several innovations in combi measurements for thin films and gradient thin films (see Table 3-2), including rapid and accurate measurement of film modulus (a measure of a material's ability to deform, such as its elasticity). Traditionally, measuring the modulus in thin films was capital and labor expensive, leading to limited measurement of this important property of polymer thin-film materials. NCMC researchers developed a film-buckling method where applied strain causes the film sample under test to buckle and create periodic wrinkles that are related to the local modulus of the polymer film. This modulus measurement technique used readily available and much less expensive materials than the traditional method (nano-indentation) and provided results quickly. The NCMC measurement technique is applicable to gradient thin films and traditional thin-film samples and can be used on soft or hard films, leading it to be adopted rapidly by many academic labs doing research on polymer thin films. Researchers previously unable to or severely restricted in measuring thin-film modulus are now able to measure modulus inexpensively over a larger number and variety of samples.

3.2 Combi Using Robotics for Discrete Sample Libraries

The NCMC used two methods of making discrete libraries: generating a gradient film sample followed by sectioning the film to create a discrete library, and using robotic dispensing systems. Commercial systems for discrete libraries already existed at the time NCMC was founded, and commercial instrument makers were continuing to develop systems useful for viscous polymer systems. Because of the existing commercial effort, NCMC tended to not focus on discrete library generation. However, discrete libraries are important to industry given their compatibility with industry's existing toolsets. This need for discrete libraries led industrial researches in combi to adapt NCMC's efforts in continuous libraries to the development of discrete libraries or to simply use NCMC's results with continuous libraries as inspiration for developing their own combi methods relevant to discrete libraries.

An example of discrete library fabrication and testing at NCMC is a study of the effect of epoxy resin and curing agent concentration on bond strength between the epoxy and a glass substrate. A matrix of droplets with varying concentrations of epoxy resin is generated like the one in Figure 3-2 using the computer-controlled system that varies concentration, mixes the components, and deposits a specified amount at each location in the matrix. Alternatively, a researcher would measure the amount of resin and curing agent for each sample, mix it by hand, and deposit it on the glass substrate.

Next the bond strength between the cured epoxy and glass is measured. NCMC developed a method of testing for edge delamination by introducing minute edge defects and cooling the substrate. Failure is observed with a digital camera and recorded. Figure 3-3 shows the type of failure map this process can generate rapidly. An application of this technology is the development of bonding adhesives in attaching chips to computer boards with the requirements of reducing material use and reducing component size while preventing failure during a range of operating conditions.

Figure 3-2. Library of Epoxy Droplets with Varying Concentration of Epoxy Resin Generated by Computer-Controlled System (Robot)
Samples were prepared by an automated system of varying component composition, inline mixing, and deposition into a matrix. Source: NIST Combinatorial Methods Center.

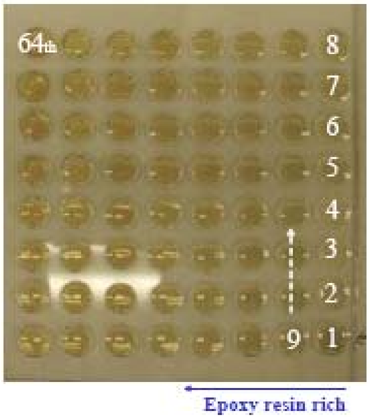
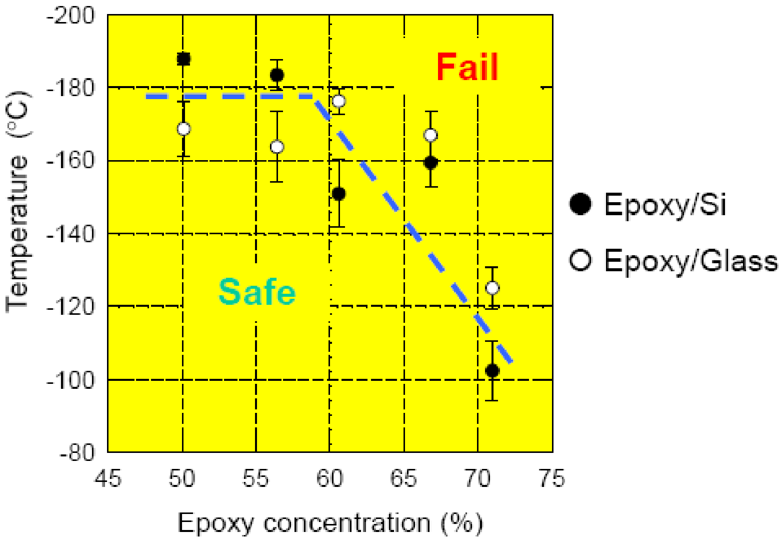


Figure 3-3. Failure Map for Varying Epoxy Concentration
Epoxy samples with varying amounts of resin and curing agent were tested for bonding with glass and silicone (Si) substrates. A failure map is readily prepared digital images taken of the library after introducing small edge defects and cooling the library. Source: NIST Combinatorial Methods Center.



3.3 Combi Using Microfluidics Libraries

Microfluidic devices are a means to manipulate small volumes of fluids in channels that are millimeters or micrometers in diameter. The advantage of using microfluidics libraries is to measure formulations across a series of changing reaction conditions, either continuously or discretely. The ability to make and handle small liquid samples reduces the amount of materials needed and produces less waste. Additionally, chemical reaction times can be reduced and heat and mass transfer times can be reduced as a result of the small scale of the devices. The small samples generated can then be analyzed for chemical composition or physical properties like viscosity and interfacial tension. The integrated discipline of making and testing samples in small flow-through devices has the goal of developing "lab on a chip" technology. That is, the process that required several researchers to have a large lab and a variety of lab equipment can be reduced to a small device that does it all.

Microfluidics is best known and widely used in the biochemistry and pharmaceutical fields as a way of making and handling small-volume aqueous samples in a continuous fashion (Sia and Whitesides, 2003). The application of microfluidics to polymer-based solutions is challenging, given that they typically require organic solvents and are more viscous than water-based systems. The high viscosity makes mixing more difficult, while the organic solvents tend to dissolve or swell materials used in making aqueous-based microfluidics systems. For example, the silicone (PDMS) devices developed by Whitesides' (Sia and Whitesides, 2003) and Quake' (Quake and Scherer, 2000) research groups are degraded by solvents typically used with polymers such as acetone or toluene. Additionally, the properties to measure are broader than those traditionally done in the biochemistry/pharmaceutical disciplines using microfluidics. NCMC pioneered concepts in fabricating inexpensive microfluidics devices with solvent resistance and using them to make gradients in samples with inline/online testing of materials properties. Currently, uptake by industry of NCMC's microfluidics for polymer combi libraries is minimal because of the incompatibility with their existing toolsets and the need to generate larger samples to meet the testing and development needs of the polymer-chemical industry. However, one industrial representative indicated that developing new formulations and polymer reactions with microfluidics is attractive because of the reduction in hazardous materials handling and waste generation, potentially making it greener and cost competitive.

NCMC developed methods to rapidly fabricate solvent-resistant fluidic devices that can produce discrete libraries of materials contained in droplets (Cygan et al., 2005). The same technology can be used to produce continuous gradient samples where the sample is either the effluent from the device or where the sample is formed/deposited on a surface contained within the device (e.g., gradient film formation).

A demonstration of the microfluidics platform to make and test a library is the UV-curing of a dental material containing monomer (reactant used to make polymers) and a crosslinker (a crosslinker connects polymers into a network, thus increasing material strength). Residual monomer in the cured compound is undesirable (could leach out in one's mouth), so curing as a function of composition needs to be studied (Barns et al., 2006). Researchers use a microfluidics device to create droplets of organics in a water-surfactant solution to make a composition library with monomer content that varies from about 10% to 100%. The droplets are then cured with UV light, and the monomer content in each droplet is measured. Figure 3-4 illustrates this type of device.

The reaction conversion (monomer remaining) needs to be measured for each droplet composition. NCMC innovated Raman spectroscopy (inelastic scattering of laser light by chemical bonds in molecules) with fiber optic collection of the data for use with a microfluidic device. Figure 3-5 illustrates the conversion of a monomer as a function of composition.

3.4 Informatics for Combi

Central to a successful combi workflow is managing the data. The large volumes of information from the contents of the library created to the results for each measurement on the library must be analyzed and correlated. Furthermore, all the data created across many libraries may provide unique results and direct future experiments. This examination of existing data across many experiments (often unrelated at the time of conception) is called data mining. The handling and analysis of the data sets from combinatorial experiments require an informatics infrastructure that integrates, manages, and helps direct the combinatorial workflow.

The NCMC developed a flexible informatics system based on open-source languages. The NCMC system addresses the challenge of handling a diverse data set of input parameters (e.g., molecular composition, structure, formulation, processing conditions) and output material properties and performance (e.g., modulus, optical properties, resistance to wear) (Cebon and

Figure 3-4. Microfluidics Device for Making Organic Phase Droplets
A discrete composition gradient of droplets is made at junction B. The monomer (benzyl methacrylate) is mixed with the crosslinker (hexanediol dimethacrylate), and the concentration of the monomer is varied by droplet as a function of distance from point B. Each droplet can function as a micro reactor for studying the effect of composition on reaction conversion. The region between A and C is the area for UV curing and Raman spectroscopy to measure conversion of the monomer. Source: NIST Combinatorial Methods Center.

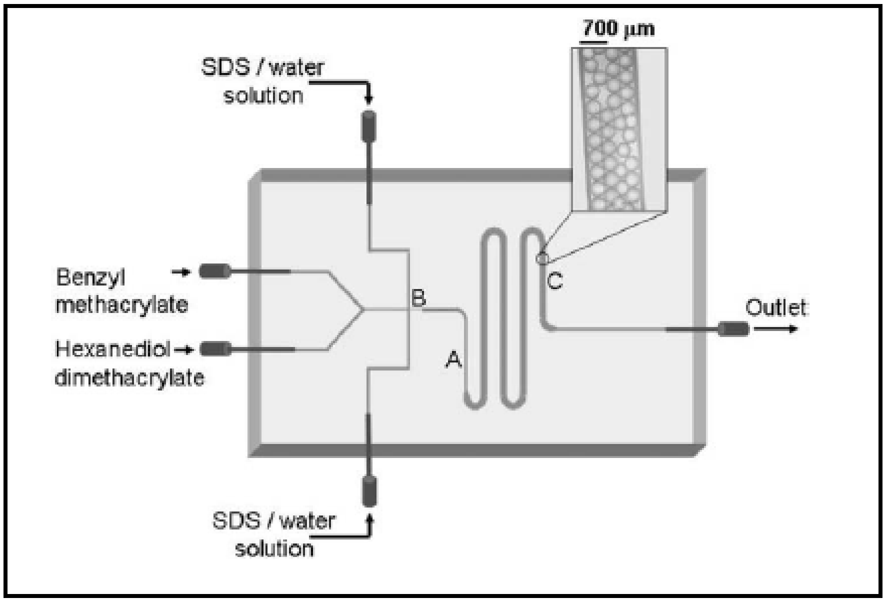
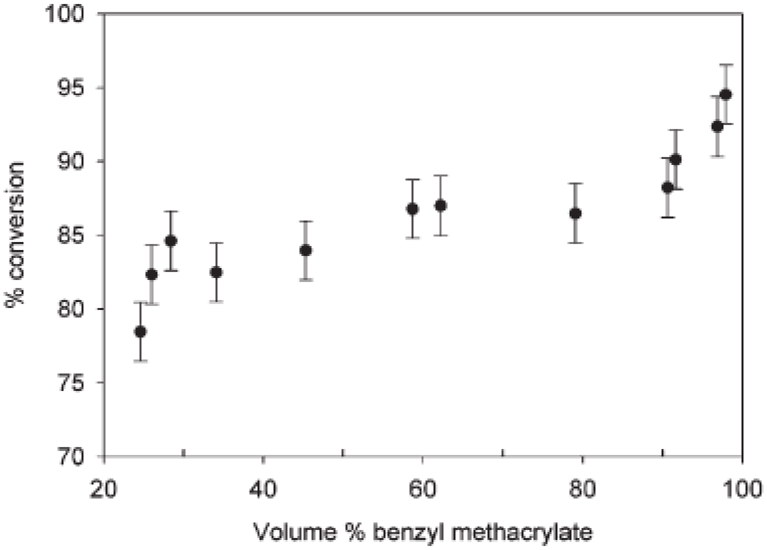


Figure 3-5. Percentage Conversion of Monomer in a Dental Material

A microfluidics device was used to prepare a gradient in a monomer (benzyl methacrylate) composition with a crosslinker. Addition of a crosslinker decreases conversion as measured in a device using Raman spectroscopy with fiber optic collection of data. Source: NIST Combinatorial Methods Center.



Ashby, 2006; Zhang et al., 2005). Although a good informatics system can be central to the success of a combinatorial effort, the handling of large and diverse data sets was already of interest to the commercial software community. A number of commercial companies have developed software packages for data handling and analysis. Since commercial software developers depend heavily on their intellectual property (IP) in software and data handling concepts, they were uninterested in endangering their IP by entangling it with public-domain work done by the NCMC. Industrial users of informatics systems require more mature and ready-to use software than that developed by the NCMC, so they purchase commercial software to meet their informatics needs. However, the Center did publish papers describing the essential aspects of informatics and held two educational workshops on their development.

4. END USERS, INDUSTRIES, AND APPLICATIONS

As an approach to screening for materials properties combi's potential crosses industries and disciplines. Research groups testing for combinations of materials properties or discovering new ones may benefit from the combinatorial or high-throughput approach if the scale of materials samples they seek to screen is sufficiently large. A thin-film temperature gradient library may allow a researcher to identify the correct thickness or materials composition, for instance, but may be in an industry wholly unrelated to those counted among NCMC members and alumni, such as someone in the R&D division of a boiler manufacturer.

To quantify economic benefits, however, we must define the end-user population along the lines of industrial classifications to extrapolate accurately the economic benefits from survey responses to national-level impact estimates. Interviews as well as a review of the science and technology literature indicated that NCMC's impacts have affected five stakeholder groups:

- advanced materials manufacturers (e.g., resins, rubber, specialty chemicals, synthetic fibers) that produce and market material components to other industrial consumers;
- paints, coatings, and adhesives manufacturers (collectively referred to as "coatings");
- personal care and household products firms that use combi to study formulations;
- academic and government laboratories that employ combi in academic research settings; and
- laboratory equipment, software, and service providers that participate in the consortium to connect with customers, participate in the technical dialog, and leverage NCMC's methods, software, concepts, and manuals.

Although this section reviews each stakeholder group individually, it is important to note that there is significant overlap between stakeholder groups at the firm level. For example, companies such as Dow Chemical produce materials components for use in other industries as well as coatings and adhesives. As a result, Dow would be considered a part of both the advanced materials and coatings stakeholder groups.

The NCMC has worked to lower the technical and financial barriers to implementing combi, but combi still requires large investments to restructure R&D workflows, train researchers, and purchase needed equipment. As a result, internal combinatorial research programs tend to be located in larger organizations. During interviews with industry representatives, it was repeatedly stated that combi tends to be concentrated in firms with net sales exceeding $1 billion per year.

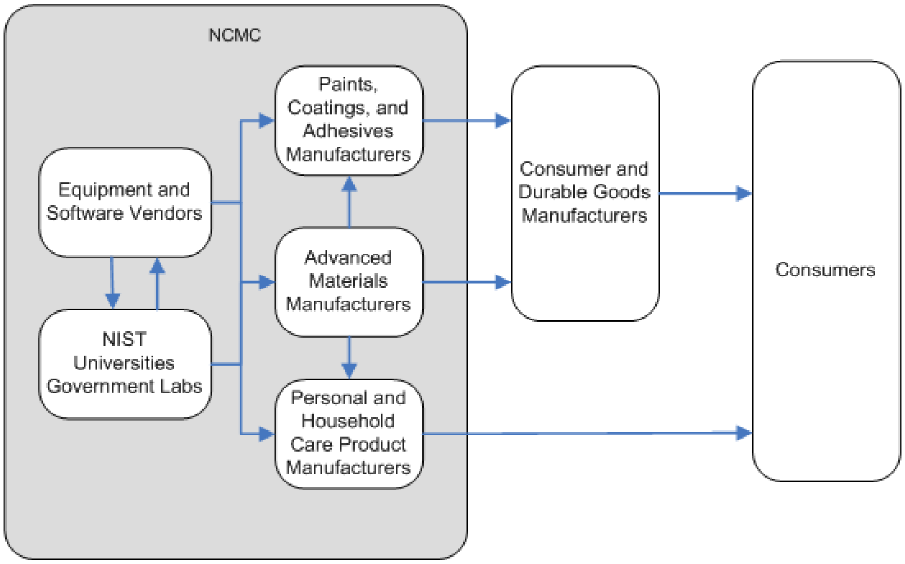
Any improvements inspired by the NCMC also have the potential to affect other stakeholders through improved knowledge, services, or equipment and software. The specific form of these benefits will differ from case to case. For example, if an equipment manufacturer develops a new tool based on one of NCMC's accomplishments, then purchasers of that equipment will benefit from increased efficiency just as the equipment manufacturer itself benefits from revenues generated through a new product line.

Improvements in the infrastructure supporting advanced materials R&D also affect companies that use polymers as inputs in their production processes. These benefits are created because polymers are used as inputs into the production of both coatings and personal care products. For example, NCMC's techniques may allow a firm in the advanced materials industry to develop a new resin that allows some coatings manufacturers to formulate coatings with improved or new properties. The benefits of the NCMC continue to flow into a broad range of consumer goods industries that are too numerous to list (see Figure 4-1). Investments in the R&D technologies and supporting infratechnologies (including combi) offer significant economies of scope in the form of large net economic benefits across many user industries and ultimately consumers.

4.1 Advanced Materials Industry

Counted among the names of firms in the advanced materials industry—a cross-section of specialty chemicals, resins, fiber, materials, and fiber companies—are some of the most familiar names in industrial chemistry: Air Products, Arkema, Bayer Materials, BASF, Dow Chemical, and Rohm & Haas, among them. Smaller firms in this intensely competitive industry are few because of the high capital intensity and high production volumes required to earn competitive returns. These firms' customers and suppliers are distributed globally as are their corporate

Figure 4-1. Simplified Flow of Benefits through the Combi-Enabled Value Chain



research divisions. Indeed, like their American counterparts, foreign companies have substantial investments in corporate research centers outside their home countries; NCMC members BASF and Bayer Materials each have large R&D centers in the United States, for instance.

Firms in the advanced materials stakeholder group manufacture a diverse range of products such as resins, rubbers, composites, and synthetic [North American Industry Classification System (NAICS) code 3252]. The products produced by firms in this stakeholder group are typically not sold to consumers. Rather they are sold to other industries where they serve as inputs into the production of other products. As a result, the products manufactured by advanced materials firms are pervasive in modern life. For example, resins are used to create plastic products ranging from water bottles to industrial-grade components. Advanced materials manufacturers provide customers with products that meet exacting properties and specifications, As a result, these firms must engage in R&D to improve existing products and discover new materials that may possess properties desired by consumers.

The pervasiveness of advanced materials products helps explain why this stakeholder group is the largest in terms of both sales and employment. In 2006, the advanced materials stakeholder group employed 78,600 workers and generated shipments valued at $95 billion (Table 4-1). Manufacturers of plastic materials and resins accounted for the vast majority of this activity, employing 69% of all workers and generating over 84% of the total value of shipments. A significant portion of the total value of shipments of advanced materials manufacturers is accounted for by sales to overseas customers. In 2006, these firms generated approximately $32 billion in exports or 34% of the total value of shipments that year. The vast majority of these exports, approximately 80%, were made by plastic material and resin manufacturers.

Chapter 1 described how the discovery, formulation, and optimization of such polymers are difficult tasks because a large number of parameters impact the properties these materials exhibit. By providing researchers with a means to synthesize polymer samples quickly across a wide parameter space, combi may allow advanced materials manufacturers to develop more quickly new or improved materials with properties that are more desirable to their customer base. In 2004, researchers at Dow published an article in *Macromolecular Rapid Communications* that described how using high-throughput equipment enabled them to evaluate these interactions in a much shorter period of time than traditional methods. The analysis time was measured in hours instead of weeks (Peil et al., 2004).

4.2 Paints, Coatings, and Adhesives Industry

Firms in the paints, coatings, and adhesives stakeholder group produce coatings that are applied to objects to improve one or more of their surface properties (e.g., appearance, adhesion, water resistance, scratch resistance). Like advanced materials, coatings are encountered frequently in everyday life, often without the knowledge of most individuals. Although coatings may be sold directly to consumers (common examples would be latex paint

Table 4-1. Descriptive Statistics for Key Combi-Adopting Industries, 2006

NAICS	Industry Description	Total Value of Shipments ($millions)	Number of Employees	U.S. Total Exports ($millions)	U.S. General Imports ($millions)	Trade Balance ($millions)
3252	**Resin, Synthetic Rubber, and Artificial Synthetic Fibers and Filaments Manufacturing**	**$94,373**	**78,557**	**$32,044**	**$14,504**	**$17,540**
325211	Plastics Material and Resin Manufacturing	$78,995	54,042	$25,751	$10,433	$15,318
325212	Synthetic Rubber Manufacturing	$6,889	8,570	$4,040	$1,600	$2,440
32522	Artificial and synthetic fibers and filaments manufacturing	$8,488	15,945	$2,253	$2,471	−$218
3255	**Paints, Coatings, and Adhesives Manufacturing**	**$32,911**	**59,628**	**$3,286**	**$1,335**	**$1,952**
32551	Paints and Coatings Manufacturing	$23,358	39,006	$1,987	$852	$1,135
32552	Adhesives Manufacturing	$9,553	20,623	$1,299	$482	$817
3256	**Soap and Other Detergent Manufacturing**	**$84,802**	**99,868**	**$9,707**	**$6,318**	**$3,389**
32561	Soap & Cleaning Compound Mfg	$40,467	44,684	4,565	2,123	$2,442
32562	Toilet Preparation Mfg	$44,335	55,184	5,143	4,196	$947

Sources: U.S. Department of Commerce, Bureau of the Census. 2007. 2006 Annual Survey of Manufactures. Obtained through American Fact Finder Database <http://factfinder.census.gov/home/saff/main.html?_lang=en>.

U.S. International Trade Commission (USITC). 2008. Interactive Tariff and Trade DataWeb. Available at <http://dataweb.usitc.gov/scripts/user_set.asp>. As obtained on May 1, 2008.

or car wax), they are more often sold to other industries as inputs into their manufacturing process. As a result, coatings are used in products individuals encounter everyday from the paints on automobiles to nonreflective coatings on television screens.

In 2006, this industry employed over 59,000 workers and generated approximately $32.9 billion in total value of shipments (Table 4-1). The vast majority of these shipments (71%) were generated by paints and coatings manufacturers, while adhesives manufacturers represented the remainder. A relatively small amount of shipments ($3.2 billion or 10% of the total value of shipments) were directed toward overseas customers.

All coatings are formulated by mixing chemical ingredients such as resins, catalysts, pigments, pigment dispersants, solvents, and other additives. Formulation is a complex process that historically has depended on experimentation for developing or improving products, thus making it a natural candidate for combi methods.

Evidence that coatings manufacturers are already adopting combinatorial methods can be found in the press releases of large chemical companies. For example, in 2006, BASF and Robert

Bosch GmbH's began developing a high-throughput screening plant to speed up the testing of pigments, resins, and additives in their coating formulations. According to Dr. Thomas Brinz, head of Bosch's "Lab Systems" division, "The ultra-modern robotic facility designed jointly with BASF allows for the first time to examine complex coating recipes from the formulation of the raw materials through to the finished coating product thoroughly in an integrated facility. Thus, depending on the requirement, up to 100 different coating systems can be processed in a very short time" (BASF, 2006).

Data on the amount of domestic R&D being conducted by coatings manufacturers is collected by NSF and aggregated with data collected for other chemical manufacturers, which in addition to coatings manufacturers included manufacturers of agriculture chemicals (NAICS 3253) such as pesticides, manufacturers of personal care and household cleaning products (NAICS 3256), and other chemicals (NAICS 3259).

4.3 Personal Care and Household Products Industry

Personal care and household products include cosmetics, perfumes, soaps, shampoos, and a variety of household cleaning solutions (NAICS code 3256). Major personal care product manufacturers include Procter & Gamble, Unilever, and Avon, all of which are current or former NCMC members. As one might expect from the familiar presence of soaps, perfumes, and other products in everyday life, personal care and household product manufacturers are the second largest of the three chemical manufacturing stakeholder groups.

In 2006, this industry generated a total value of shipments of approximately $86 billion and employed over 99,000 workers (Table 4-1). That same year, exports for this industry were valued at approximately $9.7 billion (or 11% of the total value of shipments that year).

Similar to coatings, personal care products are formulated from a variety of components that are mixed together to create their desired attributes. As a result, combinatorial methods could also increase the pace of product development. Evidence of the potential impact of combi on the development of personal and household products can be found in a 2002 interview between *Chemical & Engineering News* and Parmond Reddy (a chemist at NCMC alumnus Procter & Gamble). Dr. Reddy indicated that the work NCMC was doing on creating high-throughput methods for measuring interfacial tension was of great interest to developers of shampoos, detergents, and other cleaning products. Dr. Reddy said that interfacial tension was something researchers at Procter & Gamble "measure day in and day out." Procter & Gamble participated in NCMC's interfacial tension focus project, which NCMC initiated in response to industry comments such as Dr. Reddy's.

4.4 Academic and Government Research Laboratories

Unlike the previous stakeholder groups we have discussed, academic and government laboratories are not generally driven by a profit motive, which may lead them to pursue different types of research than research pursued by other stakeholder groups. These labs are not primarily focused on developing products but on generating basic or applied scientific knowledge for general publication or for use by their funding organizations. The benefits that these institutions receive from combi differ very little from those received by other stakeholder groups: 1) time-saving methods for synthesizing and analyzing compositions more quickly than if they did so by hand, and 2) a means to broaden the scope of research questions they are able to study.

Correspondence with individuals at NCMC and interviews with academic researchers identified at least 17 U.S. academic labs at research universities that have implemented combi workflows and likely benefited from NCMC's technical accomplishments. NSF surveys academic institutions annually to determine the size and scope of their research activities. A list of the 17 institutions and their 2006 R&D expenditures in the physical sciences and engineering disciplines are provided in Table 4-2.. The list primarily includes institutions that are known to have implemented significant combi workflows in their labs. This information is presented for informational purposes only; it is not known how much R&D is making use of combi at these institutions.

Other institutions without combi workflows may also be using NCMC technical methods, especially gradient thin-film or microfluidics techniques. Similarly, we are also not likely aware of all the labs that have adopted combi workflows.

In addition to academic institutions, other institutional laboratories may be affected by the NCMC. One prominent example is NCMC alumnus Wright-Patterson Air Force Base (formerly known as the Air Force Research Laboratory), which is dedicated to leading the discovery, development, and integration of military technologies. Also, the Lawrence Berkeley National Laboratory in California conducts nonclassified materials research that may have been affected by NCMC's technical achievements.

4.5 Equipment and Software Vendors

Combinatorial research techniques require the use of tools that can create large amounts of sample compounds and quickly analyze their properties. These tools include physical equipment used for synthesizing samples and performing tests, as well as the software used to run these machines and to analyze the results they generate. Manufacturers of these tools represent an important factor in making combinatorial techniques accessible to researchers.

As stated previously, equipment vendors like Symyx that were members of the consortium may benefit less from technical accomplishments generated by the NCMC because their market is in discrete sample libraries. Vendors may also focus on other kinds of materials, but even if polymers were not their primary interest, participating in the center assisted in their endeavors related to combi. However, manufacturers of discrete libraries may still benefit from the NCMC because it offers a venue for interacting with potential clients and staying up to date on research and market trends.

Table 4-2. Research Institutions Conducting Combinatorial Materials Research, 2006

Institution	Total R&D Funding ($thousands)	Physical Science R&D Funding ($thousands)	Engineering R&D Funding ($thousands)	Metallurgical/ Materials Engineering R&D Funding ($thousands)
Arizona State University	201,955	19,051	71,479	5,082
Clarkson University	16,143	N/A	N/A	N/A
Clemson University	179,840	10,376	81,309	14,815
Georgia Institute of Technology	440,898	35,570	294,466	14,286
Iowa State University	221,998	11,010	51,726	4,976
Massachusetts Institute of Technology	600,748	98,367	220,043	17,320
North Carolina State University	330,936	22,189	96,066	8,237
North Dakota State University	103,778	14,355	10,557	N/A
Princeton University	188,165	28,357	55,548	20,796
Rutgers University	308,204	39,420	25,245	5,957
Texas A&M University	492,955	38,430	161,735	5,750
University of Colorado, all campuses	512,794	63,594	36,721	N/A
University of Massachusetts, Amherst	136,057	29,363	28,301	N/A
University of Pittsburgh	530,162	19,109	21,254	3,071
University of Wisconsin, Madison	831,895	55,697	92,933	5,272
University of Maryland, College Park	354,244	60,990	88,321	6,040
University of Southern Mississippi	39,163	9,907	1,313	N/A

Source: National Science Foundation. 2007. "Academic Research and Development Expenditures: Fiscal Year 2006." Available at <http://www.nsf.gov/statistics/nsf08300/>. As obtained on May 11, 2008.

Manufacturers of other types of equipment, such as equipment used for high-throughput measurements, might use NCMC technology in certain aspects of product development. For example, equipment manufacturers apply coatings to certain parts of their equipment. NCMC techniques could be used to determine how thickly they should apply the coating if another parameter such as temperature is involved.

Equipment and software vendors are spread across several NAICS codes and make up only a small portion of each. To determine which firms were active in the equipment and software stakeholder group, RTI searched the published literature. Table 4-3 lists the equipment and software vending companies RTI identified. This table reports each company's sales, employment, R&D expenditures, and whether they provide equipment, software, research services, or a combination of the three.

Table 4-3. Equipment and Software Vendors for Combinatorial Workflows

Company	Location	Sales ($millions)	Employees	R&D Expenditures ($millions)	Equipment (E), Software (S), Services (V)
Accelrys Inc.	San Diego, CA	$81	372		S
Amtec GmbH	Chemnitz, Germany				E
Anton Paar GmbH	Graz, Austria				E
Avantium Technologies	Amsterdam, The Netherlands				E, S, V
Biotage AB	Uppsala, Sweden	$1,175	332	$629	E
Brookfield Engineering Laboratories, Inc.	Middleboro, MA				E
Bruker Corporation	Billerica, MA	$548	1,905	$50	E,V
CambridgeSoft Corporation	Cambridge, MA	$9	65		S, V
Chemspeed Technologies	August, Switzerland				E,V
HEL Group	Hertfordshire, UK				E, V
hte Aktiengesellschaft	Heidelberg, Germany	$7	60		P
Hysitron, Inc.	Eden Prairie, MN	$4	57		E
J-KEM Scientific	St. Louis, MO	$1	18		E
Jobin Yvon Inc	Edison, NH	$50	211		E
Mettler-Toledo	Greifensee, Switzerland	$1,595	9,100	$83	E
nScrypt	Orlando, FL				E
Symyx Technologies, Inc.	Santa Clara, CA	$125	380	$66	E, S, V
Tecan Inc.	Maennedorf, Switzerland	$333	1,087		E
Varian Inc	Palo Alto, CA	$835	3,700	$60	E, V
Veeco Instruments Inc	Woodbury, NY	$441	1,279	$63	E
Waters Corporation	Milford, MA	$1,280	4,687	$77	E, S
Zinsser Analytic GmbH	Frankfurt, Germany	$6	33		E

Source: Company Forms 10-k and Hoovers.com.

5. STUDY METHODOLOGY

The NCMC introduced novel combi technologies and demonstrated combi's utility, invigorating interest in and accelerating combi's adoption for R&D in organic polymers. In some cases, interviewees believe these advances would not have occurred for 5 or more years (if at all), and the technologies that would have ultimately come to market might have been substantially more expensive.

The most common comment during stakeholder interviews was that the NCMC demonstrated what was possible with combi, which then catalyzed innovation within corporate research divisions and academic labs. Some NCMC technologies were adopted with little additional customization; others were adapted or influenced the development of custom systems that otherwise would not have existed. The consortium offered a coordinated technical community—both with semiannual members' meetings and at large ACS and MRS conferences—in which researchers tasked with leading their firms' efforts in high-throughput R&D strategy were able to interact with their peers and learn from NIST's experts.

Our approach to valuing economic impacts was to prepare a series of counterfactual analyses that linked hypotheses about the NCMC's benefits to relevant technical and economic metrics. These metrics then informed processes for collecting data and estimating measures of economic benefit. Benefits were estimated against a scenario in which the NCMC did not exist and key advances in thin films and microfluidics libraries were not made.

5.1 Conceptualizing NCMC's Role and Economic Benefits

The total economic impacts of infratechnology development and consortium programs such as the NCMC can be broken out into five distinct categories:

- *technology adoption/adaption*: the benefits of adopting new technologies or adapting them to suit an organization's purpose
- *knowledge base expansion*: the benefits of acquiring technical information and data that improve an organization's knowledge base
- *consortium experience*: the benefits of membership in narrowly defined forums in which all respondents are focused on a single technical topic
- *downstream product cost and quality*: improved quality of goods and services in which those materials are an input and that potentially reduce the costs of those goods and services
- *time acceleration effects*: accelerated the accrual of cost savings or product quality benefits for end users

In economic analyses such as this one, each component of the total economic impact will generally have elements that are more tangible than others. The first three bullets pertain to R&D efficiency: acquiring infratechnology and knowledge that permit researchers to do more with less. NCMC methods and “how-to’s” for adapting common laboratory apparatus to perform high-throughput experiments and enable end users to accrue labor, material, and capital cost savings over the life of the project, relative to the defending manual one-at-a-time methods. Cost savings from the introduction of a new technology in a process can be calculated by comparing total costs for one period with those observed in a previous period. Those benefits are realized, meaning that they have accrued and are measurable. In this retrospective economic impact analysis, the study’s focus was on the NCMC’s realized benefits, which we compared with historical observed costs. Some NCMC technology has yet to be adopted and there is the possibility that this technology may hold benefits for end users in the future.

Stakeholders also could not quantify downstream product quality benefits or end-user acceleration benefits. Quantification is very difficult, although it is likely that benefits do exist. Combi has directly affected key materials in many products, but these ingredients are combined with many others in a wide variety of products from shampoos to semiconductor devices to the hulls of cargo ships. These products’ performance is affected by work flowing out of the NCMC. What proportion of their net economic value is attributable to or was accelerated by combi was not sufficiently distinct to be quantifiable.

For example, one interviewee said that “several” products her company markets were affected by combi in some way, but she declined to articulate how they were affected and to what extent NCMC innovations may have played a role in their development because the information is proprietary. Given that a portion of the NCMC’s economic value was not quantified, but most costs were captured, the net economic benefits and measures of economic return are conservative.

5.2 Theoretical Approach to Estimating Economic Benefits

This study quantified R&D efficiency benefits and acceleration benefits for organizations using combi. We estimated both the economic impact of combi in general and the portion of that economic impact attributable to the NCMC’s introduction of novel NCMC technologies. Acceleration benefits include the benefits for firms adopting combi earlier than they otherwise would have.

5.2.1 Modeling Economic Impacts of the NCMC’s Contributions to Combi

A recurrent theme in this report is that NIST’s contributions to combi are characteristic of generic technologies and infratechnologies. The technologies are generic because the suite of systems presented in Chapter 3 present functional concepts of how common laboratory instrumentation can be adapted or new apparatus can inexpensively assembled to implement combi. NCMC’s contributions in terms of technical approach, fabrication techniques, and a system of measurement are infratechnologies because they are foundational to the use of combi for thin films and microfluidics.

The increase in economic welfare from using combi is the benefits accruing to combi adopters from more efficient and effective R&D and the benefits accruing to end users from producing products whose features, cost, and/or quality are enhanced by materials emerging from combi-enabled R&D. End users would be companies purchasing a polymer product for input in their production process.

The preceding section highlighted the challenges to measuring materials end-users benefits accurately. However, by developing representative firm R&D and production cost functions for combi adopters under the current and counterfactual conditions, we can measure the benefits accruing to them to develop a lower-bound estimate of combi's impacts. Understanding the mechanism through which costs are incurred and benefits may accrue is essential to developing the taxonomy of costs and benefits underlying this analysis. It should be noted here that many combi end users are academic and government laboratories, but the discussion of how NCMC-developed technology benefits firms is also applicable to them.

Combi's immediate impacts are on the combi-adopting firm's R&D costs: changes in the proportions of and costs of capital, labor, materials, and technology consumed during materials research. Industry-level impacts are the sum of impacts accruing to all firms composing the industry. Identifying the appropriate technical and economic impact metrics, measuring them relative to a counterfactual scenario, and extrapolating results from a survey sample to the industry population yields economic benefits. These benefits must, however, be reduced by the programs' costs.

A time series of net economic benefits would therefore be:

$$
\begin{aligned}
\Delta \text{ net economic benefits}_t = \; & (\textstyle\sum \Delta \text{ R\&D capital savings}_{it} + \\
& \textstyle\sum \Delta \text{ R\&D labor savings}_{it} + \\
& \textstyle\sum \Delta \text{ R\&D materials savings}_{it}) - \\
& (\textstyle\sum \Delta \text{ technology acquisition costs}_{it} + \\
& \textstyle\sum \text{NCMC program costs}_{it})
\end{aligned}
$$

It is also possible that one R&D output is a new polymer product that is more cost-effective to produce. Thus, production costs may change. The new polymer product may also be of higher quality or have a suite of novel properties, in which case it could possibly command a higher price 'in the market or sell more units'. If the firm was a price taker, as is common in bulk commodity industries, there may be no change in price. Beyond this conceptual view, and in practice, the model must reflect comments from scoping interviews with industry: appreciable differences in price, quantity, and production costs, though possible, were not disclosed by the real-world firms participating in the study.

5.2.2 Accelerating Combi Adoption

The above discussion of modeling firm-level economic benefits did not consider the time dimension. The time value of money means that a dollar is worth more today than tomorrow and accelerating the time series of economic benefits generates value. Thus, measuring the economic impact of combi overall was necessary to accurately assess the extent to which NCMC influenced the adoption of combi, regardless of whether a firm adopted any of the NCMC's generic technology.

The top portion of Figure 5-1 illustrates a stylized flow of costs and benefits from the perspective of the combi-adopting firm relative to not using combi. Costs accrue for implementing a combi workflow, but those costs are expected to be recouped by cost savings or profits over time. Traditional investment theory states that if the net present value (NPV) of the flow of benefits is greater than zero, then the company will undertake the investment project subject to a budget constraint. The NCMC's mission was to accelerate combi adoption in addition to developing novel, cost-effective tools for combi adopters.

The potential impact of NIST on users' costs and benefits is shown in Figure 5-1. NIST's contributions have

(a) reduced combi workflow development and acquisition costs and time: these cost reductions are shown by the shaded square area. Time reductions are shown as a shift in the curve to the left.

(b) reduced combi workflow implementation costs and time: the cost reductions are reflected in the nonparallel shift in the implementation stage.

Combined, the two time reductions shift the entire life-cycle curve to the left by time "t" resulting in the acceleration of benefits shown in the second shaded area of the lower portion of Figure 5-1.

Figure 5-2 illustrates the adoption of combi over time. The vertical axis indicates the cumulative share of adoptions through a given year, and the horizontal axis is time. Because adopting combi is not a discrete event and adoption grows over time, market adoption is modeled as a continuous diffusion curve. The S-shaped diffusion curve approaches the full industry potential asymptotically.

Figure 5-1. Firm-Level Acceleration of Costs and Benefits

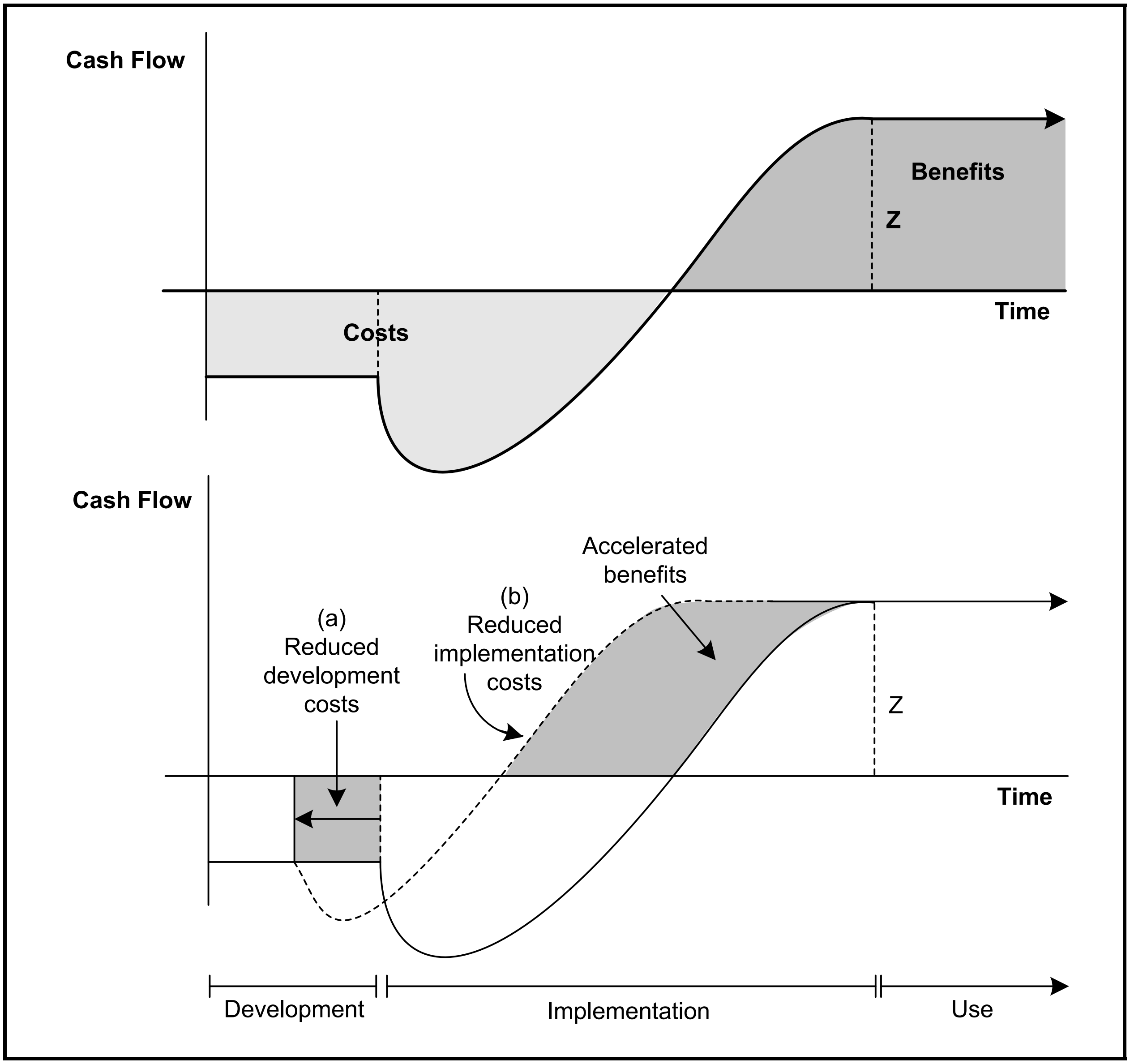
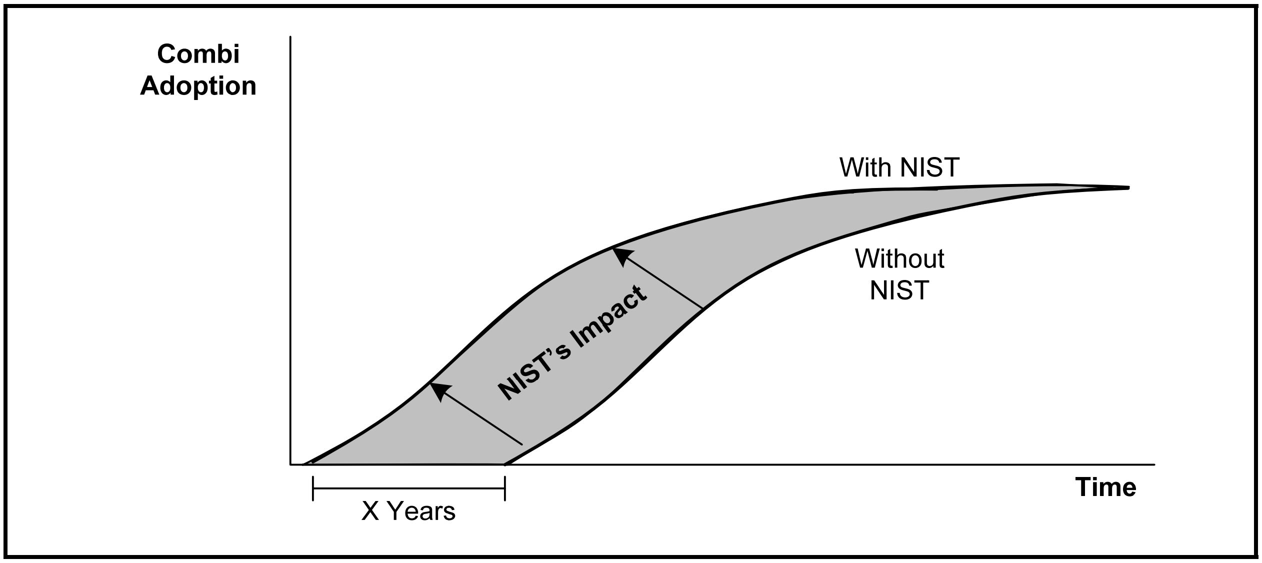


Figure 5-2. NIST's Acceleration Effect on Combi Adoption



Forecasting combi's rate of diffusion is challenging because it is in the early stages of adoption. It is a function of the number of current adopters, the number of potential adopters, and the rate at which information and knowledge pass from one agent to another. This study forecasts diffusion using an S-shaped logistic curve. Originally, only a small number of firms adopt this technology. As more firms observe the benefits realized by initial adopters, they too adopt the technology.

5.3 Specifying the Counterfactual Scenario without the NCMC

Today some research laboratories are using combi that otherwise would not because of NIST's program. NIST's contributions to microfluidics and thin-films research were particularly disruptive. Symyx and other vendors were offering comparable and, in some cases, more sophisticated technologies for discrete libraries, but NIST was the leader in thin films and microfluidics for polymers. Interviewees believe it would have taken from 5 to 10 years before comparable, inexpensive strategies for thin films would have been devised without NIST's contribution.

The counterfactual scenario against which benefits were measured specified that

- the novel suite of techniques for gradient approaches to thin films and elements of microfluidics and discrete sample library combi would not have been available before 2008 and firms would have incurred greater capital, materials, and labor expenses as a consequence;
- the overall adoption rate of combi for organic polymers would have been lower, meaning that some users' adoption likely would not have occurred until years later;

- the costs of adopting combi would have been higher, and some laboratories would not have been using combi at all; and
- the absence of the NCMC as a consortium hampered information diffusion and offered no coordinated forums for discussion of the development of the combi toolkit for organic polymers, particularly for thin films and microfluidics.

While NCMC did not invent combi, it accelerated combi's adoption through its outreach work in the technical community, demonstrating what was possible with combi and reducing and/or eliminating cost barriers, thus making it more cost-effective on an ongoing basis. To ease the information collection burden on survey respondents, we "packaged" all of NCMC's technical accomplishments into a general combi toolkit that was a subset of the broader combi toolkit. We assessed acceleration and efficiency benefits for both combi overall and the NCMC toolkit.

Exceptional research centers for combi development and combi applications in discrete libraries existed at universities such as North Dakota State University. However, these centers relied on corporate funding and were subject to CRADAs. Thus, in addition to their focus on combi for discrete libraries, the free flow of information outside of these centers could not have been a substitute for the NCMC.

The value NCMC members, visitors, and alumni derived from the consortium experience, such as networking and marketing among peers, would not have occurred. In addition to these informal exchanges, training and productivity benefits from more formal exchanges, such as meetings and demonstrations, would not have occurred. The broader community would not have benefited from papers, how-to's, proceedings, and demonstrations emerging from the Center.

5.4 Taxonomy of Quantifiable Economic Benefits and Costs

In this section, we offer the specific categories of benefits and costs as well as the technical and economic metric pairs used to measure and monetize them. Table 5-1 presents an overview of the taxonomy of costs and benefits analyzed in this study.

5.4.1 Value of Consortium Experience

NCMC members often cited the consortium experience as one of the key benefit categories for RTI to investigate. The consensus view among interviewees was that one of the primary benefits of the NCMC was networking and engaging with other researchers in a precompetitive environment sponsored by a governmental group. Researchers stated that company policies and the presence of competitor firms often make it difficult for them to engage in substantive conversations in a group environment. At NCMC meetings researchers were able to connect with other researchers working on similar problems one on one. This was possible because the NCMC focused on precompetitive research and topics. In other words, participation in the NCMC, and the amount of feedback and information NCMC collected as a consequence, was possible in part because of NCMC's choice to center discussion on generic and emerging

Table 5-1. Summary Taxonomy of Quantifiable Benefits, Acquisition Costs, and NIST Costs

Benefit	Description	Benefit Components	Adoption Cost Components	NIST Cost Components
Consortium experience	NCMC hosts researchers and provides an environment for networking and informal exchange with leading firms applying combi on a precompetitive basis	*NCMC Members:* ▪ Marketing benefits ▪ Transactions benefits ▪ Recruitment benefits ▪ Preferential access ▪ Researcher training ▪ Demonstrations ▪	*NCMC Members:* ▪ Membership fees ▪ In-kind expenses ▪ Labor participation ▪ Travel costs	▪ Program administration ▪ Technical program costs ▪ Facilities investment ▪ Conference participation and organization ▪ Miscellaneous costs
Knowledge base expansion	NCMC presentations, technical documentation, data, and analytical results	*All Beneficiaries:* ▪ Validation of research strategies ▪ Avoided essential research • New research methods		
Technology adoption	NCMC-developed or -brokered techniques and strategies enable efficiencies in R&D and accelerate product development	*NCMC Members:* ▪ Focus project research *All Beneficiaries:* ▪ Workflow design ▪ Reduced capital expense ▪ Labor efficiency ▪ Materials efficiency ▪ Accelerated product development	*NCMC Members:* ▪ Focus project fees *All Beneficiaries:* ▪ Equipment and materials ▪ Toolkit development ▪ Installation ▪ Training ▪	

materials classes and methods development rather than exact materials types and specific measurement solutions.

Many members interviewed believed that the NCMC improved technology transfer *among* researchers as well as from the NCMC *to* researchers. One interviewee noted that “one of the biggest advantages of working with NIST is that you’re working with a group of very smart people that are far more advanced in terms of where you are on the learning curve from measurement aspects.” What respondents also found to be compelling was that the Center was more practically focused than most academic consortia. They viewed the costs of participation as low, the reputation of NIST as a neutral partner as a key success factor, and being part of the community as having substantial tacit benefits.

We identified four broad categories to capture the benefits from the exchanges within the consortium model (see Table 5-2):

Table 5-2. Benefits Metrics to Capture the Value of the Consortium Experience

Benefit Category	Specific Cost	Technical Metric	Economic Metric
NCMC meeting researcher training and demonstrations	Labor costs	Labor hours for acquiring comparable technical knowledge from secondary resources	Loaded hourly wage rate for scientists participating in the consortium
	Labor costs	Labor hours expended on developing comparable training sessions	Loaded hourly wage rate for scientists participating in the consortium
Marketing and networking benefits	Labor costs	Labor hours for achieving comparable visibility and awareness among peers	Loaded hourly wage rate for senior scientists participating in the consortium
	Travel expenses	Estimated associated travel needs to achieve visibility and awareness	Estimated travel expenses
	Conference fees	Estimated comparable conference attendance for achieving the same	Estimated conference fees
Recruitment benefits	Labor costs	Labor hours expended to identify similarly qualified employment candidates	Loaded hourly wage rate for senior scientists participating in the consortium
	Labor costs	Labor hours to bring non-NCMC postdoc candidate to equivalent skill level	Loaded hourly wage rate for recent postdoc hires
Transactions benefits	Labor costs	Incremental labor hours otherwise expended to facilitate transactions among NCMC members in the absence of the consortium	Loaded hourly wage rate for senior scientists participating in the consortium

Note: RTI used wage-rate estimates from the Bureau of Labor Statistics' (BLS') Occupational Employment Survey to 1) enhance repeatability of our results and 2) reduce the information collection burden on interviewees. According to the BLS, the average annual salary, excluding benefits, for a materials scientist engaged in scientific research and development services was $84,790 in 2007. The hourly wage estimate was multiplied by 2 to account for fringe, administrative, and overhead expenses.

- training benefits from hands-on demonstrations, presentations from leading researchers, and discussion series;
- marketing and networking benefits stemming from participation in an industry consortium dedicated solely to combi for organic polymers;
- recruitment benefits associated with hiring an NCMC postdoc with hands-on NCMC training as opposed to researchers without that experience and investing in their training; and

- transactions benefits associated with interactions among potential customers, teaming partners, and collaborators.

5.4.2 Value of Knowledge Base Expansion

Members often mentioned that although some concepts and methodologies developed in the NCMC did have a specific application within their organization, the knowledge they gained from observing these advances was beneficial. For example, research projects or presentations from invited lecturers at semiannual meetings may have offered insights that enabled the researchers to overcome a technical obstacle similar to what was discussed in the consortium or invalidated an internal technology proposal that would not have born fruit.

There is a training benefit to the NCMC that is difficult to duplicate elsewhere. Most members stated that the training value of being party to the Center was alone worth the annual membership fee. Similar benefits included learning new methods and viewing demonstrations of novel combi approaches (including apparatus design and protocols).

The NCMC assists the combi community by providing essential research, offering insights into key focus projects, and validating research strategies. Access to NCMC prepublications permits members to learn about new techniques before they enter the public domain. The broader technical community benefits from NCMC innovations (how-to's, technical papers, software, data), but members have access to this information more than 1 year before the broader community does.

In the words of one member, the NCMC has a "ripple effect" within R&D labs: the research they perform yields knowledge that validates or invalidates research strategies. The member said that they learned that one of their research projects would fail before they started the project and, thus, assigned the resources to more promising work.

We identified three broad categories to capture the benefits from the formal exchanges within the consortium model (see Table 5-3):

- researcher training benefits stem from the NCMC's core mission to educate researchers on adopting and implementing a combinatorial workflow in their R&D labs through publications and presentations; these benefits accrue to the consumers of the NCMC's technical output who may be NCMC members or nonmembers;
- avoidance of basic research expenditures that accrue from leveraging NCMC knowledge, thereby avoiding labor, capital, and materials spending; and
- validation or invalidation of research strategies, which leads to greater R&D efficiency.

Table 5-3. Benefits Metrics to Capture Value of Knowledge Base Expansion

Benefit Category	Specific Cost	Technical Metric	Economic Metric
Researcher training	Labor costs	Labor hours for acquiring comparable technical knowledge from secondary resources	Loaded hourly wage rate for scientists participating in the consortium
	Labor costs	Labor hours expended on developing comparable training sessions	Loaded hourly wage rate for recent postdoc hires
Avoided research	Labor costs	Avoided labor hour expenditure on foundational research	Loaded hourly wage rate for senior scientists participating in the consortium
	Materials costs	Avoided materials purchases	Estimated materials costs
	Capital costs	Avoided equipment purchases and depreciation on basic research	Estimated equipment costs
Validation of research strategies	Labor costs	Avoided labor hour expenditures on strategies that the NCMC disproved; efficiency gains from identifying the correct approach initially	Loaded hourly wage rate for scientists participating in the consortium
	Materials costs	Avoided materials purchases	Estimated materials costs
	Capital costs	Avoided equipment purchases and depreciation on basic research	Estimated equipment costs

5.4.3 Value of Technology Adoption and Adaptation

The NCMC introduced novel technologies in combi workflows and accelerated others. Respondents in our scoping interviews stated that although “off-the-shelf” solutions to several NCMC innovations existed, the cost advantages of the NCMC approaches enabled a wider variety of laboratories to adopt combi. NCMC technologies have one-time cost advantages (e.g., equipment and set-up) and ongoing savings.

Combi allows researchers to miniaturize experiments (less material, less waste) and reduce the number of tests performed (less time). Moreover, continuous libraries permit nearly infinite internal analysis of a sample space, something that could not be done otherwise. Scoping interview respondents stated that combi offers a 10- to 25-fold improvement in time efficiency versus hand preparing and analyzing individual samples, and that cost savings mostly stem from time savings. The benefits categories for technology adoption and adaptation are in the same structure as the preceding two benefits discussions: labor, capital, and materials. We want to capture the economic value of less material, less waste, and less equipment expense (see Table 5-4).

5.4.4 Technology Acquisition Costs

All costs borne by all non-NIST groups fall into a broad category called technology acquisition costs. Technology acquisition cost is a contra account to benefits because the benefits firms accrue are offset by costs for consortium fees, training and travel expenses, and equipment expenditures, for example. While the surveys may request end users to provide measures of benefit net of cost, an accurate taxonomy of adoption cost categories is needed to illustrate the magnitude of investment needed to derive quantified benefits.

Technology adoption cost categories encompass

- NCMC membership fees and focus project cost shares;
- labor expenses for NCMC meeting attendance and focus project research;
- in-kind labor, materials, and equipment expenses in lieu of other NCMC contributions;
- travel and conference expenses; and
- direct labor, materials, and equipment expenditures to adopt or adapt NCMC technology.

5.4.5 NCMC and Tool Development Costs

MSEL management provided financial data on the NCMC for the program dating from early 2002 when the Center was first created. These data were supplemented with information on the costs from the pioneering research in thin-films libraries.

Table 5-4. Benefits Metrics to Capture the Value of Technology Adoption

Benefit Category	Specific Cost	Technical Metric	Economic Metric
Productivity	Labor costs	Incremental labor expenditure to acquire equivalent data volumes from other sources	Loaded hourly wage rate for scientists participating in the consortium
Training	Labor costs	Avoided training on dedicated equipment that may have otherwise been purchased	Loaded hourly wage rate for scientists participating in the consortium
Materials usage optimization	Materials costs	Incremental materials consumed to acquire equivalent data volumes	Estimated materials costs
	Materials disposal costs	Avoided hazardous waste disposal costs	Estimated disposal costs
Avoided capital expenditures	Capital costs	Avoided dedicated equipment purchases and installation	Estimated equipment costs

5.5 Time Period of Analysis

Choosing a time frame for estimating the economic impacts of such technological improvements can be difficult because there are potentially long and variable lags between commencing a research activity and generating an improvement in technology (Alston et al., 1995). Even after research leads to a technological improvement, several years may pass before the technology begins generating benefits through its adoption. A simplified illustration of this process of development and adoption is provided in Figure 5-1.

When thin-films library research began at NIST in 1998, applying combinatorial methods to polymers was a relatively new field of research—the first paper describing such an application was published only the previous year in 1997 (Brocchini et al., 1997). As a result, there were no commercially available instruments or published techniques for creating libraries of polymer samples, yet these methods had great potential for industry applications. NIST's Polymers Division responded to this need by investing in fundamental research that centered on creating a foundation for practical applications of combi for materials discovery.

The period of analysis begins in 1998, the year in which Eric Amis, Alamigir Karim, Carson Meredith, and others at NIST began developing gradient thin-film libraries, and ends in 2007, the last calendar year for which full-year NCMC financial data are available. Scoping interviews with end users suggested that thin-film libraries account for a significant proportion of economic benefits. It is important to capture the costs associated with those technical advances; therefore, the period of analysis begins 4 years prior to the official launch of the NCMC in 2002.

The results of NIST's research were first presented in 1999 at the Gordon Conference on Reactive Polymers, Ion Exchange, and Adsorbents (Meredith et al., 1999) and were ultimately published in a series of papers in 2000 (Meredith et al., 2000; Meredith, Karim, and Amis, 2000). This marked the beginning of when stakeholders in private companies and academic research labs could begin adopting or adapting the techniques NIST developed in their own research.

5.6 Primary Data Collection

Data informing this analysis were collected from semistructured interviews, survey forms completed via e-mail and returned to RTI, and an Internet survey of materials discovery scientists. Most responding scientists were employed by NCMC members or alumni, research universities, or large chemical companies that did not join the NCMC. All were directly involved in polymers R&D.

Primary data collection efforts were conducted in three phases:[2]

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[2] The formal data collection surveys in this analysis were approved by OMB as well as RTI's Institutional Review Board.

- Phase I consisted of scoping interviews over a wide range of topics with researchers from the NCMC, its member and alumni companies, and academic researchers. The purpose of the scoping interviews was to explore combi and its impacts to inform hypotheses about the NCMC's economic benefits. RTI researchers also attended the NCMC-13 meeting.
- Phase II was the distribution of the survey forms that could either be completed on the Internet (https://combisurvey.rti.org) or via e-mail using an electronic form. We used two forms: one for NCMC members and alumni (Appendix B) and one for the broader community (Appendix C). To maximize distribution of our survey announcements, we partnered with the MRS, which placed survey announcements in their members' newsletter, "Materials360," and distributed a link via ACS's Polymers Group Listserv.
- Phase III was predominantly a series of follow-up interviews with respondents to either the member or the nonmember survey. A limited number of supplemental scoping interviews were also conducted to verify our assessment and synthesis of data from Phase II.

This study respected the sensitive nature of the information provided by respondents needed to quantify economic benefits. As a philosophy of high-throughput experimentation, combi is central to firms' R&D strategy. We endeavored to work with companies to get approvals for their researchers' participation in this analysis given that our focus was on the benefits of combi and not the substantive content of their research strategies. Respondents were promised confidentiality and that only aggregated data would be presented in the report. Respondents to the Internet survey had the option to respond anonymously.

5.7 Extrapolation to National Impact Estimates

Results from the survey sample were extrapolated to national estimates using publicly reported R&D expenditures for firms in the advanced materials, paints and coatings, and personal and household care product industries that are likely to be using combinatorial methods in their research. Sales and employment data are traditionally used to extrapolate benefits, but as combi resides in the R&D function, and the percentage of R&D effort related to combi is the most accurate measure of activity.

The challenge to extrapolation presented by combi is that it is an approach applicable to multiple research settings in multiple industries. For the period of interest, however it is generally believed that adoption by industry has been highly concentrated in a small number of industries and by firms of a certain size class within those industries. As described in Section 4, an industry representative revealed that the firms most likely to be using combi in these industries have net sales exceeding $1 billion per year. Therefore, to create an extrapolation base RTI used the Hoovers industry database to identify all public companies with either direct or secondary business lines in manufacturing advanced materials, paints & coatings, and personal care products with sales exceeding $1 billion per year in 2007. We also included all current and former NCMC members. After the first pass at assembling the basket of representative companies that would serve as the core R&D base, we added key foreign and domestic companies that both have US R&D operations and that fit the profile of a likely target combi adopter. The inclusion of some foreign firms in the extrapolation base was important given that they maintain significant R&D operations in the U.S. The firms comprising the extrapolation base are listed in Appendix A.

RTI thoroughly quality checked this list of companies to ensure that the companies included were relevant for the purposes of this study. After this quality checking was complete, RTI utilized the COMPUSTAT North American database to collect annual revenue and R&D expenditure data for these companies from 1998 to 2007.

Given the sensitivity in querying companies about their R&D activities and expenditures, the survey requested firms to provide their stock ticker or their publicly-report R&D budgets. RTI aggregated benefits for all survey respondents and then used the ratio of this benefits total to their aggregated R&D budgets to generate national impact estimates. Chapter 6 provides a summary table of the extrapolation base.

Note that a firm's inclusion in R&D base does not mean that they use combi or participated in this analysis. Rather, the extrapolation base was created first with current or former NCMC members and then augmented according to the screening criteria outlined above. It is also possible that a survey respondent outside of the given criteria was not included as part of the extrapolation base because the extrapolation base was to be publicly reported.

RTI did not extrapolate benefits from consortium-specific measurements to national impact measurements. These benefits accrued only to current and past NCMC members and were measured solely from a census of all members and alumni. RTI did, however, extrapolate benefits pertaining to technology adoption, adaption, and knowledge base expansion, which were not limited to NCMC members.

5.8 Measures of Economic Return

Three benchmark measures—benefit-to-cost ratio (BCR), NPV, and internal rate of return (IRR)—were used to evaluate the time series of quantified benefits and costs.

Benefit-to-Cost Ratio

The BCR calculated in this analysis is the ratio of the NPV of benefits to the NPV of costs, which accounts for differences in the timing of cash flows (which has implications for the real value of $1 in one time period versus another).

Letting B_t be the benefits accrued in year *t* by firms and C_t the total costs for the project in year *t* by NIST, then the BCR for the program is given by

$$(\mathrm{BCR}) = \frac{\sum_{i=0}^{n} \frac{B1_{(t+i)}}{(1+r)^{i}} + \sum_{i=0}^{n} \frac{B2_{(t+i)}}{(1+r)^{i}}}{\sum_{i=0}^{n} \frac{C_{(t+i)}}{(1+r)^{i}}} \tag{5.1}$$

where

t is the first year in which benefits or costs occur,

n is the number of years the benefits and/or costs occur, and

r is the social discount rate.

In this study, *r* was set at 7%, the Office of Management and Budget (OMB)-specified level.[3] Because benefits and costs occur at different time periods, both are expressed in present-value terms before the ratio is calculated. Essentially, a BCR greater than 1 indicates that quantified benefits outweigh the calculated costs. A BCR less than 1 indicates that costs exceeded benefits, and a BCR equal to 1 means that the project broke even.

Net Present Value

The NPV of the investment in a project is calculated as

$$NPV = \sum_{i=0}^{n} \left[\frac{B1_{(t+i)}}{(1+r)^{i}} + \frac{B2_{(t+i)}}{(1+r)^{i}} - \frac{C_{(t+i)}}{(1+r)^{i}} \right], \tag{5.2}$$

where the terms have the same meanings as identified for Equation (5.1). Any project that yields a positive NPV is considered economically successful. Projects that show a positive NPV when analyzed using OMB's 7% real discount rate are socially advantageous. A negative NPV would indicate that the costs to society outweigh the benefits, and an NPV equal to zero would indicate a breakeven point.

Internal Rate of Return

The IRR on an investment should be interpreted as the percentage yield on an R&D project over the life of the project, often multiple years. In mathematical terms, the IRR is the value of r that sets the NPV equal to zero in Equation (5.2) or results in a benefit-cost ratio of 1 in Equation (5.1).

The IRR's value can be compared with conventional rates of return for comparable or alternative investments. Risk-free capital investments such as government bonds can be expected to yield rates of return under 5% in real terms, while equities seldom return more than 10% over an extended period of time. In academic studies of the diffusion of new technologies, however, real rates of return of 100% or more have been found for significant advances with

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[3] See OMB Circular A-94.

broad social benefits (Tassey, 2003). It should be noted that, in cases for which costs exceed benefits, an IRR cannot be calculated.

6. NET ECONOMIC BENEFIT ESTIMATES

This chapter presents quantified net economic benefit estimates attributable to the NCMC of

- participating in the NCMC consortium,
- expanding the combi knowledge base,
- introducing novel technologies, and
- accelerating many firms' adoption of combi and HTE.

The research divisions of many coatings, materials, and personal care and household products firms provided the data and contextual information that made it possible to quantify estimates and assess the NCMC's contribution to combi and materials science. Almost all private-sector survey respondents fell into these industry groups. Their responses were augmented by contributions from academic researchers, equipment and software vendors, and government researchers. Some respondents completed survey instruments and participated in multiple rounds of informational interviews. More than 70 researchers participated via surveys, telephone interviews, or in-person discussions.

Figure 6-1 compares study respondents' publicly reported R&D expenditures to the total estimated R&D expenditures for firms in the affected industry segments with annual sales greater than $1 billion.[4] As discussed in Chapters 4 and 5, combi is still in the early stage of adoption for polymers R&D, and most firms currently using combi are large publicly traded firms. Only two firms with annual sales below $1 billion responded to the survey. Respondents to our survey had publicly reported R&D expenditures of $29.2 billion, which was equivalent to 72% of the total R&D expenditure estimated for combi users in the industries covered by this analysis.

Quantified benefits in this chapter are conservative for four principal reasons. First, we were only able to reliably quantify impacts for early combi adopters and adopting industries. Adoption of NCMC combi technology outside of the materials, coatings, and personal care and household products industries could not be estimated. Economic benefits accruing to other industries were not quantified. Second, as presented in Chapter 5, benefits for industries that use combi-enabled polymers and benefits for the final end user that accrues quality or performance benefits from polymer-containing products could not be quantified. Third, benefits for two stakeholder groups, equipment vendors and academic laboratories, could not be reliably estimated.

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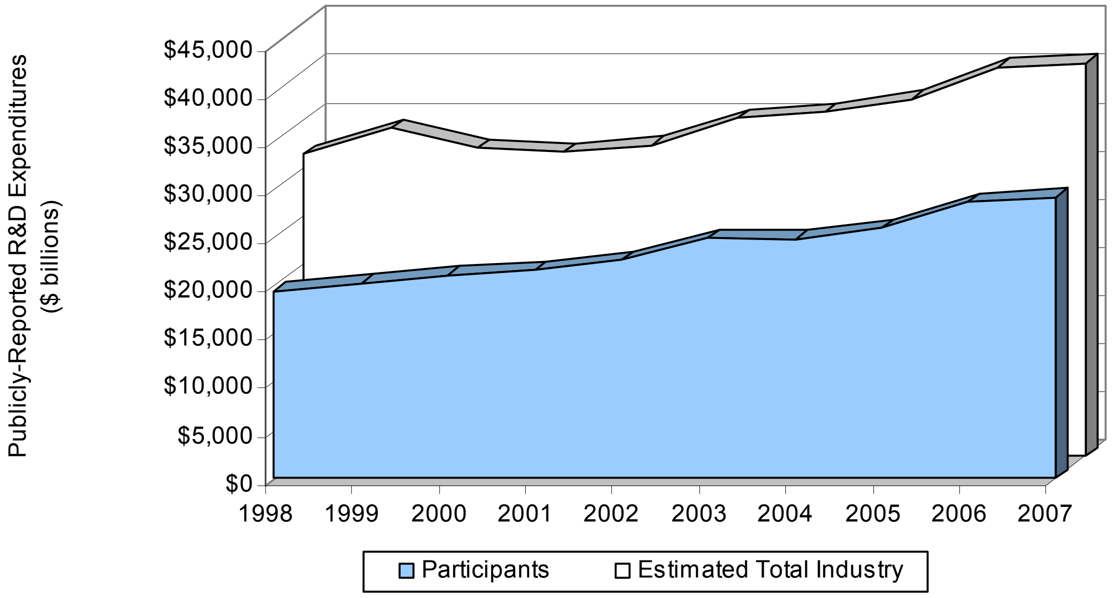
[4] As stated in Chapter 5, relevant R&D expenditure data used for extrapolating estimates to national benefit estimates was the sum of R&D expenditures by all firms in the affected industries with revenues greater than $1 billion. We refer to this group of firms as the affected industry segment because industry experts predicted that firms in smaller size classes are not likely to be using combi at this time. The decision to use publicly reported R&D budgets as the extrapolation measure was in response to the extreme care necessary when exploring the R&D activities of firms in highly competitive industries.

Figure 6-1. Survey Participation as a Proportion of Total Industry Publicly Reported R&D Expenditures



Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. Appendix A lists the firms whose R&D expenditures compose the total estimated expenditures for firms with sales greater than $1 billion in materials, coatings, and/or personal and household care products industries. Also included in the estimate are current and former NCMC members. The rationale underlying firm selection is presented in Chapter 5.

Many of the same types of benefits accruing to industry researchers also accrue to academic ones. Several academic researchers cited cost and time savings relative to earlier sample preparation and analysis methods when applying NCMC combi technology. Although academic respondents stated that they used the NCMC approaches infrequently, when applied, those approaches offered efficiency benefits. Fourth, combi's adoption is ongoing, and in addition to unquantified benefits detailed above, there are benefits beyond 2007 that have yet to accrue and were also not estimated.

6.1 Respondent Profile and Combi Usage History

This section complements Figure 6-1 and profiles survey respondents and their reported combi usage. Seventy-four percent of respondents reported that they used combi or that they had used it in the past. Of those who reported not using combi, 60% expect to use it in the future. Respondents who have not used combi were exited from the survey after being offered the opportunity to comment on why they did or did not expect to use combi in the future. Those who expected to use combi cited that lower costs and a maturation of how to use combi polymers made the approach more attractive relative to other methods. Respondents who did not expect to use combi almost uniformly stated that combinatorial approaches were not well suited for their research.

Two respondents reported suspending their combi program because of difficulties in applying these methods or because they believed the costs were too high relative to the benefits they were accruing or had expected to accrue. Other interviewees reported that several firms encountered challenges with adopting and integrating combinatorial workflows in the early 2000s. Indeed, some NCMC members' decision to join the consortium was in part to learn from other firms' and NIST's experiences. Eighty percent of members and alumni joined the NCMC as part of their combi adoption strategy. The remaining 20% joined to interact and network with researchers and to stay abreast of trends in combi (see Table 6-1).

On average, respondents reported becoming aware of the successful, practical use of combi in late 2001 and began using it between 5 and 6 years ago (see Table 6-2). Members and nonmembers reported learning about advances in combi for polymers through presentations at MRS, ACS, Gordon Conferences, and the Knowledge Foundation. They also reported learning about combi through the technical literature and through direct interactions with NIST researchers. A small number of firms were developing their own combi techniques and programs for discrete sample libraries in the late 1990s, making them very early adopters. Their research coincided with NIST's early research into thin films libraries.

Table 6-1. Respondents' Combi and HTE Use

Survey Question	Yes	No
Does your company or university research laboratory(-ies) currently use combi or HTE for polymers R&D, or has it used combi in the past?	74%	26%
If <u>no</u>, do you expect to use combi in the future?	60%	40%
Did your company join the NCMC as part of a combi adoption plan (NCMC members survey only)?	80%	20%

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

Table 6-2. Timing of Respondents' Combi Adoption

Survey Question: "In which year(s) would you estimate that the following occurred?"	Mean	Range
Researchers in our lab became aware of the successful, practical use of combi for polymers R&D	2002	1997–2007
My lab(s) implemented and began using combi for the first time	2003	1997–2008
Combi became a part of the regularly-used methods in our lab(s)	2004	1997–2009

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

During interviews several members stated that they would have preferred the NCMC to do more research and toolkit development in discrete sample libraries since this library type was most common. Yet, as mentioned earlier in this report, discrete sample libraries benefited from an established commercial infrastructure, and NIST's goals were to expand and demonstrate the viability of combi for new materials systems using low-infrastructure gradient thin film and microfluidic methods. Thus, there was some degree of disconnect between the stated interests of industry in desiring greater NCMC research on specific systems, and NIST's mission of bridging technology gaps by focusing on more general demonstrative cases. NCMC members without interests in future research directions ceased participation and transitioned to alumni status. Despite the apparent disconnect, NCMC continued to attract new members, and alumni stated that they derived value from their membership but that their research interests no longer aligned with NCMC's agenda.

Figure 6-3 presents a time series of full-time equivalents (FTEs) respondents reported tasking with developing and applying combi.[5] The data in this figure provide insight into the pattern of combi adoption. The data suggest that the amount of person effort expended to develop combi among respondents is declining and that a greater amount of effort is devoted to applying combi. Overall, the effort expended developing and adopting combi workflows exceeded the labor expended applying those methods in ongoing research activities until 2005. The run up in combi development activities was largely between 2000 and 2005, which is consistent with the combi adoption timing reported in Table 6-2.

6.2 Economic Benefits of the NCMC Consortium Experience

The first major component of the NCMC's economic benefit we sought to quantify was that of participating in the NCMC consortium itself. During early interviews, members indicated that their participation offered more productive marketing and networking opportunities with other researchers in combi than other conference opportunities. Consequently, the survey asked NCMC members and alumni to reflect on the benefit of partnering with NIST and participating in the NCMC.

Results show that participating in the consortium, whose meetings were attended by 30 to 50 industry researchers plus invited guests and NIST staff, was reported as being of significant benefit (see Table 6-3). The consortium offered valuable demonstration and training opportunities that enabled them to keep more readily abreast of the latest in combi-related research. They were also able to acquire information on novel approaches and inexpensive strategies for incorporating them into their workflows. On an annualized basis, 78% of members and alumni stated that the benefit of participating was equal to or greater than the membership fees paid. Half indicated that the NCMC validated internal research strategies or invalidated strategies that would not have born fruit.

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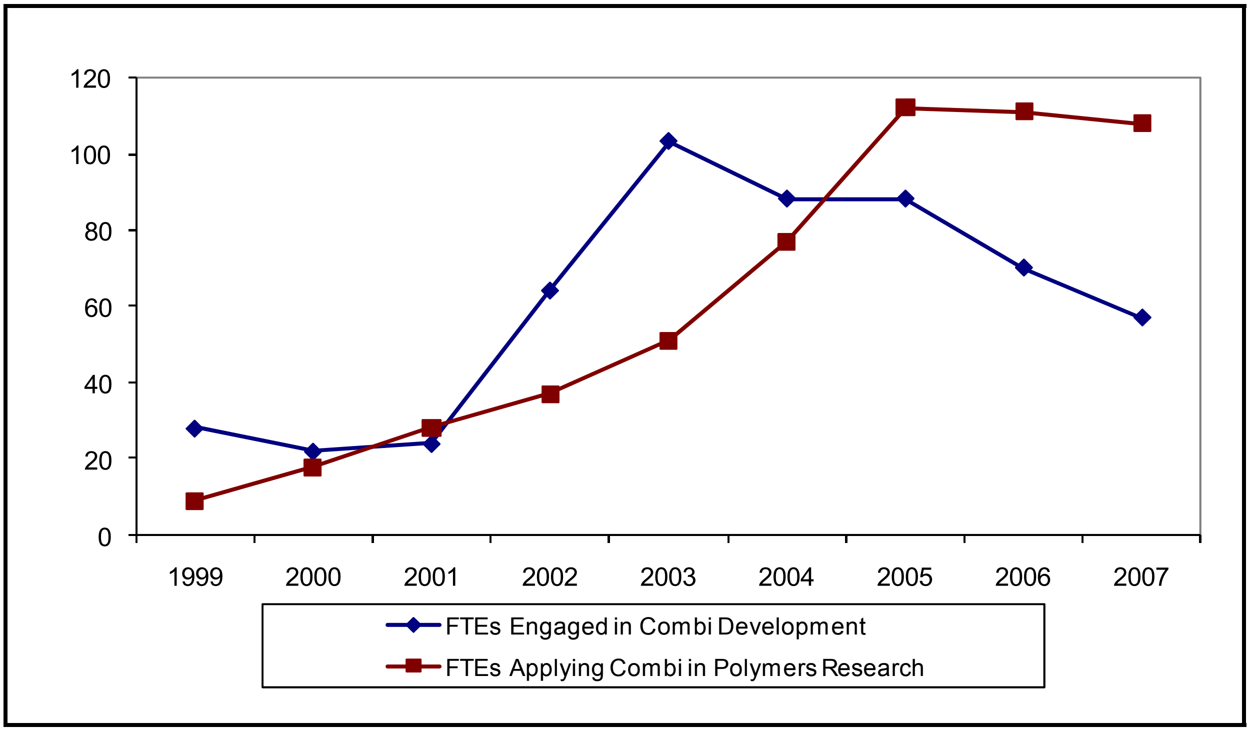
[5] One FTE is equal to 2,000 person-hours of effort (i.e., not one person).

Figure 6-3. Estimated FTEs Developing and Applying Combi in the Advanced Materials, Coatings, and Personal Care and Household Products Industries



Note: Data are in FTEs for stated industries only. The data represent FTEs and not the number of persons who may use combi overall within these industrial sectors. Equivalent data for other industries and for academia could not be estimated reliably.

Table 6-3. NCMC Members' Perceptions of the Benefits of Membership

Survey Question	Yes	No
Was the annual benefit your organization accrued from participation in the NCMC equal to or greater than the annual membership fees paid?	78%	22%
Did participation in the NCMC … offer more productive marketing or networking opportunities, relative to other conferences or combi meetings?	83%	17%
… validate or invalidate internal research projects and permit more efficient and effective resource allocation?	50%	50%
… help your organization avoid any research activities, or enable your organization to acquire needed research more quickly or cost-effectively?	70%	30%
… offer valuable researcher training and demonstrations beyond what would have been available elsewhere?	67%	33%

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

A former NCMC member commented that “the greatest benefit NCMC provided was a regular forum for combi materials outside of commercial vendors, which helped provide technology and competitive awareness [as well as] discussion and networking opportunities within the combi materials community.”

Another member noted that “the biggest benefit we have gained from NCMC is the ability to see the internals of complete ‘combi’ procedures, not just the finished product. So, by being a member of NCMC we have been able to see a project being defined, problems being identified and solutions being developed—equally the handling of samples and information from the beginning to the end of an experimental process—unlike the snapshots seen via commercial interactions.”

Two consortium benefits were quantified: (1) demonstration and training benefits from attendance at semiannual meetings and (2) hosted researcher training benefits. Interviewees told us that these semiannual meetings offered more productive networking and marketing opportunities than other combi conferences. However, we were unable to quantify these benefits.

Each of the 12 semiannual meetings held between 2002 and 2007 had a theme, and noted researchers were invited to present their research pursuant to that theme (see Chapter 2). Two additional NCMC meetings in 2008 were excluded because they fell outside of the analysis period. Common among all meetings were technology demonstrations and discussion series about emerging technical challenges.

Meetings were attended by 355 member representatives. Members estimated the typical additional person-hour effort that would have been required to derive the same value as they actually accrued from these meetings to be between 25 and 32 hours per meeting per attendee.[6] All reported hours in this analysis were quantified using the mean hourly wage for materials scientists in research and development ($40.76 [BLS, 2007])), which was then multiplied by 2 to estimate fringe and administrative expenses. The total benefit between 2002 and 2007 was estimated to be about $850,000.

NCMC also hosted visiting researchers from member and partner organizations. The benefit of the training was estimated in a similar fashion as the consortium participation benefits above—savings of the additional person-effort that would have been required to achieve the same level of knowledge and sophistication. Interviews indicated that the additional training investment would have been equivalent to the length of stay at NCMC. Thus, annual benefits were the sum of the product of the wage rate above and the estimated number of days NCMC hosted a

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[6] Individual members responded for their estimated person-hour benefits for the meetings their representatives attended. Data were extrapolated to all attendees using the ratio of responding members who attended the meeting to all NCMC member attendees. Consequently, there is some variation in the annual benefit per attendee.

researcher. NCMC records indicate that the Center offered hosted researchers 455 training days, which therefore amounted to a benefit of $286,000.

In addition to the benefit stream presented in Table 6-4, NCMC graduated postdocs to industry and academia who received 2 years of specialized combi training and were integral to the NCMC's efforts to develop the combi knowledge base. One former postdoc working with a NCMC alumnus posited that the net benefit accruing to their hire was equivalent to about 8 months to 1 year of additional training (see Chapter 2). In all, more than 25 postdocs have completed 2-year positions and are now working in industry, academia, and government.

6.3 Economic Benefits of NCMC's Expansion of the Combi Knowledge Base

The second component of economic benefits quantified was NCMC's contributions to the expansion of the body of knowledge foundational to implementing and using combinatorial approaches. The survey presented respondents with a list of technologies developed by the NCMC and its industry partners and asked whether they

- directly used or adapted the technology;
- were aware of the technology, but the technology was not relevant to their research agenda; or
- were unaware of the technology.

Recall that because NCMC technology is generic and infrastructural, some researchers may adapt it to suit their particular needs. Thus, rather than ask users whether they adopted a technology, the survey asked whether they used or adapted it.

Table 6-4. Economic Benefits of the NCMC Consortium Experience

Year	NCMC Meeting Industry Attendees (persons)	Hosted Researchers (hosted days)	Semiannual Meeting Demonstration and Training Benefits ($thousands)	Hosted Researcher Training Benefits ($thousands)	Total ($thousands)
2002	58	130	124	—	124
2003	78	157	209	85	294
2004	64	58	164	102	266
2005	48	85	114	38	151
2006	55	8	130	55	186
2007	52	7	108	5	113
Total	**355 persons**	**445 days**	**$849**	**$286**	**$1,134**

Note: All dollar values are real 2007 dollars. Sums may not add to totals due to independent rounding.

Respondents' views are presented in Table 6-5. The data show that gradient combinatorial methods for polymer thin films, NIST's leading and most substantial contribution to the field, were reported as being both the most used or adapted technology as well as the one with which respondents were most familiar. There also appears to be a high level of awareness of NCMC's contributions to the combi knowledge base.

Data provided by respondents indicate that the economic benefit of NCMC's contributions to the combi knowledge base totaled nearly $24.4 million over the period from 2001 to 2007 (see Table 6-6). These information acquisition benefits reflect two distinct advantages that accrued to end users. First, NCMC's papers and presentations invalidated some firms' research strategies, enabling them to avoid expending resources on projects that either would have ultimately failed or that would not have been as effective and efficient as those the NCMC published. Second, respondents stated that they acquired valuable knowledge about combi in general and about specific approaches. One researcher noted that although his lab had not implemented any of the methods developed by the NCMC, the overall body of knowledge that the consortium generated offered valuable insights into implementing and employing combinatorial approaches.

Table 6-5. Respondents' Adoption and Awareness of NCMC Combi Technology

Respondents' Use of the Following Methods and Technologies Developed by the NCMC and its Industry Members (% of respondents):	Use or Adapted	Aware of but Not Relevant	Unaware of Technology
Continuous thin films with gradients in temperature, composition, thickness, surface energy, or on chemically patterned substrates	45%	55%	0%
Discrete libraries used with gradients in temperature, surface energy, or thickness	32%	55%	5%
High-throughput measurement of morphology	27%	41%	23%
Buckling method of modulus measurement for thin films and soft materials	23%	64%	9%
Edge lift-off test for interfacial adhesion	23%	64%	9%
Microfluidics produced organic solvent-based libraries	14%	64%	14%
Multilens contact test for adhesion	5%	77%	9%
Interfacial tension measurement via microfluidics	5%	77%	9%
Integrated metrology (morphology, composition, extent of reaction) on microfluidics produced organic solvent-based libraries	0%	73%	18%

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

Table 6-6. Economic Benefits of Expanding the Combi Knowledge Base

Year	Labor Benefits ($thousands)	Materials Benefits ($thousands)	Capital Benefits ($thousands)	Total ($thousands)
2001		—	103	103
2002	419	30	109	558
2003	725	27	4,016	4,768
2004	859	29	4,094	4,981
2005	354	28	4,424	4,806
2006	658	26	4,228	4,912
2007	423	24	3,859	4,306
Total	**$3,437**	**$164**	**$20,833**	**$24,434**

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. Sums may not add to totals due to rounding.

The majority of knowledge-base benefits were reported to be capital expenditure savings. In interviews with researchers, we posed questions about why benefits from consuming NCMC research were largely capital savings. Interviewees told us that they were readily able to quantify avoided expenditures from implementing the NCMC approach, which often used existing or less expensive equipment. That is, researchers reported saving thousands of dollars on equipment whose purchase was precluded by published NCMC research. Those same researchers generally could not quantify approximately how much labor effort was also saved because most labor savings were considered from actually using the NCMC methods.[7]

6.4 Economic Benefit of NCMC Combi Technology and Accelerating Combi's Adoption

The final component of economic benefits was the benefit of adopting NCMC combi technology and the economic benefit from accelerating firms' combi adoption. In the case of methods developed by NCMC, the study valued the introduction of novel technology that otherwise would not have been introduced within this study's period of analysis. Some firms also reported accruing acceleration benefits attributable to the NCMC. R&D efficiency benefits accrued to firms who adopted combi earlier than they would have in the absence of NCMC's industry outreach work and publications. Where firms reported that their adoption of combi was accelerated, the firms' net benefits from the acceleration effect were included in the benefits estimate.

First, economic benefits from adopting NCMC-developed technology were quantified by measuring the cost savings from using NCMC approaches rather than the next best alternative ("defending") method. Table 6-5 lists the technologies that were presented to respondents, who

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[7] The reported average labor benefit was about 0.7 FTE (Range: 0 to 2 FTE) distributed over a 2- to 4-year period.

were then asked to compare how use of these approaches offered R&D efficiency benefits compared to alternative approaches. Productivity gains were defined as increases in the number of equivalent samples analyzed per day per researcher. Economic benefits were the value of the increase in throughput and the volume of information acquired for equivalent or lower labor, materials, or capital expenditures.

As an illustration of how NCMC's research generated economic benefits, one researcher offered the following anecdote. Her laboratory developed a new apparatus for testing the mechanical properties of small samples that was heavily influenced by methods NCMC had developed. The apparatus and its associated techniques enabled her lab to complete the research faster and at lower cost. The researcher speculated that they would not have undertaken what proved to be a highly successful project without the NCMC technology because it would have taken 10 times longer and have been 10 times more expensive.

Another respondent said that using the temperature gradient approach for thin films permitted her to do in one experiment what would normally take 25 experiments. She said that, assuming each experiment used to require 15 minutes, she can now accomplish in 30 minutes (an additional 15 minutes was required for sample preparation using the NCMC method) what would have taken her 375 minutes.

Over 90% of respondents reported that the NCMC technologies offered efficiency benefits over the technologies that they had been using before, and a slightly higher percentage reported that these technologies also enabled them to test across a broader range of samples (see Table 6-7). NCMC technology also improved the effectiveness of their R&D: 92% of respondents cited that NCMC technology improved the quality of their research and/or products that their company may produce.

One firm credited NCMC's research with assisting with the development of advanced formulation systems they use in their coatings research. While it was not a direct transfer of technology from NCMC to the firm, they did say that they would not have been able to develop the formulation system or something similar without having had the benefit of NCMC research.

Table 6-7. Respondents' Perceptions of Efficiency and Effectiveness Gains from NCMC-Developed Combi Technology

Survey Question	Yes	No
Did the NCMC-developed technologies		
… offer efficiency benefits or cost savings over what your lab had been using heretofore?	91%	9%
… enable you to test samples across a broader range of conditions?	92%	8%
… improve the quality of your research or any products that your company may produce?	92%	8%

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

The formulation system was installed in each of the firms' R&D labs, and they estimate savings to date of several million dollars relative to if they had installed commercially available formulators.

Table 6-8 presents the average reported labor productivity gains for using combi in polymers R&D in general and for using the NCMC-developed technology. The mean labor productivity gain reported from combi overall (i.e., not from only NCMC approaches) was about 8.5 fold, with individual responses ranging between 1.5 and 24 fold. The mean reported labor productivity gain for NCMC-developed approaches was 5.2 fold, with individual responses ranging between 1.2 and 12.5 fold. Follow-up interviews to explore the wide variation in reported gains suggested that the variation was attributable to differences in the techniques different labs applied, properties and materials of interest, and required rate of automation, for example.

The work performed by NCMC on microfluidics for measuring interfacial tension helped another firm develop its own microfluidic equipment. This equipment enabled his lab to perform tests up to 3 times faster compared to the previous method while using fewer materials (1 microliter of fluid using this new method was equivalent to the 100 ml of fluid required by traditional interfacial tension tests). Less labor was required because sample preparation was largely automated. Working with smaller samples had an important environmental benefit because the smaller samples size reduced waste, which, in turn, reduced hazardous material disposal costs.

The edge lift-off test for interfacial adhesion was credited for enabling another firm to analyze 5 times more combinations of parameters than had been possible with previous methods. Although they did not cite significant gains in throughput, the method did permit them to study their samples more thoroughly. As a consequence, the firm believes that their customers have more robust products, which they went on to explain meant that even if their customers did not follow their instructions to the letter, the material would still give them the desired behavior.

Many labs reported using combi approaches within some stages of their research projects and did not use a "classical" combinatorial workflow such as that presented in Chapter 1. This

Table 6-8. NCMC Acceleration of and Estimated Productivity Gain from Combi

Measure	Value
Mean overall net labor productivity gain from using combi for polymers R&D, where applicable	8.5 fold (Range: 1.5 to 24 fold)
Mean reported net labor productivity gain from using NCMC-developed technologies for polymers R&D, where applicable	5.2 fold (Range: 1.2 to 12.5 fold)
Percent of respondents reporting that NCMC accelerated their adoption of combi for polymers R&D	50%
Mean number of years respondents reported that NCMC accelerated their combi adoption	2.3 years (Range: 1 to 5 years)

Source: "Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers" Survey.

finding, taken in conjunction with the technical and economic measures discussed above, is consistent with the view that combi's benefits are best conceptualized as the knowledge that combi generates and not just on the number of additional samples that can be analyzed (Fasolka and Amis, 2007).

Half of all respondents reported that NCMC accelerated their adoption of combi by an average of 2.3 years. Some reported that their adoption of combi was accelerated by 4 or 5 years. A recurring theme was that interaction with NIST researchers gave firms more confidence in their decision to proceed with investments in combi programs. The publicity and attention NCMC drew to combi made it easier for some researchers to convince senior executives within their organizations to invest in combinatorial approaches because NCMC and NIST demonstrated that a reputable institution had successfully performed combi for polymers.

Acceleration benefits were quantified by applying respondents' reported productivity gains from combi overall to their reported FTEs using combi, subtracting adoption costs associated with FTEs developing combi and other expenses as well as any benefits from using NCMC technology. The net benefits for the reported period of acceleration were attributed to NCMC. The data in Table 6-9 illustrate that the NCMC spurred adoption most during 2003 and 2004 and again in 2006 and 2007.

Total technology adoption benefits were nearly $185 million for the materials, coatings, and adhesives industries alone. These benefits are conservative because

- not all impact categories were quantified, such as end-user benefits from improved materials;

Table 6-9. Acceleration and Adoption Benefits of NCMC Combi Technologies

Year	Benefits of Accelerating Combi Adoption ($thousands)	Benefits of NCMC-Developed Technologies			Total ($thousands)
		Labor ($thousands)	Materials ($thousands)	Capital ($thousands)	
2002		10,814	98		10,912
2003	3,857	27,246	92	154	31,349
2004	8,345	32,753	92	151	41,344
2005	1,532	35,536	86	212	37,366
2006	2,206	31,220	112	37	33,575
2007	3,142	27,046	105		30,293
Total	**$19,082**	**$164,616**	**$585**	**$556**	**$184,839**

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. Sums may not add to totals due to rounding.

- the extrapolation methodology was based on a profile of likely combi adopters within three industries;
- benefits for academic laboratories could not be reliably quantified; and
- combi's adoption is ongoing, and in addition to benefits in other industries, benefits beyond 2007 have yet to accrue and therefore remain unquantified.

6.5 NCMC Program Costs and End User Technology Acquisition Costs

Total NIST costs from 1998 to 2007 were approximately $14.5 million (see Table 6-10). These costs were augmented by NCMC membership and focus project fees of around $1 million and technology acquisition costs for NCMC-developed technology of about $7.5 million, including capital and initial labor expenditures. One respondent commented that in their experience the cost of implementing NCMC techniques was on par with some of their internally developed techniques and about half that of commercial combi vendors. Another respondent "…found the NCMC to be a good place for high-throughput ideas or approaches. The challenge was to modify their approaches to accommodate industrially-relevant materials." Low technology adoption costs relative to benefits may have been reported because many NCMC approaches used equipment that was already available in industrial laboratories. Additional capital expenditures were reported to be as little as $5,000 from some firms and as high as $300,000 for others.

Table 6-10. NCMC Program and Technology Acquisition Costs

Year	NIST Costs ($thousands)	Membership Fees ($thousands)	Technology Acquisition Costs ($thousands)	Total ($thousands)
1998	286			286
1999	495			495
2000	556			556
2001	2,266			2,266
2002	1,548	19	968	2,535
2003	1,793	153	1,219	3,166
2004	1,759	313	1,336	3,409
2005	2,420	157	1,543	4,120
2006	2,062	183	1,561	3,806
2007	1,339	214	865	2,418
Total	**$14,525**	**$1,040**	**$7,492**	**$23,057**

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. Sums may not add to totals due to rounding.

6.6 Summary Economic Benefit Estimates and Measures of Return

Table 6-11 assembles the complete time series of quantified costs and benefits for 1998 through 2007. Total benefits were over $210.4 million for the advanced materials, coatings, and personal and household care products industries. Inclusive of NIST, NCMC member, and technology acquisition costs net benefits were $187.4 million. The vast majority of benefits accrued from using NCMC-developed technologies, but the knowledge base expansion benefits equivalent to more than 10% of total benefits are equally as significant. These less tangible benefits are essentially a slice of the minimum alternative development cost for the technologies that NCMC developed for the equivalent of $23 million, and part of that $23 million included costs for administration and outreach work.

The net present value (NPV) of net benefits was $118.0 million applying the OMB-approved discount rate of 7% (see Table 6-12). The benefit-to-cost ratio, which is the ratio of the NPV of total benefits to that of costs, was estimated to be 8.55. In other words, for every $1 that NIST and its partners invested in the NCMC at least $8.55 in benefits accrued to the three industries.

The internal rate of return (IRR) was estimated to be 161%. Because the results of NCMC activities are widely used by many companies and other organizations, they have what economists call “public-good” content. In such cases, the IRR is called the “social rate of return”. In academic studies of the diffusion of new technologies, IRRs of 100% or more have been found for significant advances with broad social benefits. Based on a variety of economic studies, the hurdle rate for rationalizing such public-good investments is in the 30−50% range. Thus, the NCMC returned at least three times what would be considered the minimum acceptable IRR (Tassey, 2003).

Table 6-11. Net Quantified Economic Benefits of the NCMC

Year	Consortium Experience ($thousands)	Knowledge Base Expansion ($thousands)	Technology Adoption & Acceleration ($thousands)	Total Benefits ($thousands)	Total Costs ($thousands)	Net Benefits ($thousands)
1998					(286)	(286)
1999					(495)	(495)
2000					(556)	(556)
2001		103		103	(2,266)	(2,164)
2002	124	558	10,912	11,594	(2,535)	9,059
2003	294	4,768	31,349	36,411	(3,166)	33,245
2004	266	4,981	41,344	46,591	(3,409)	43,182
2005	151	4,806	37,366	42,323	(4,120)	38,203
2006	186	4,912	33,575	38,673	(3,806)	34,867
2007	113	4,306	30,293	34,713	(2,418)	32,295
Total	**$1,134**	**$24,434**	**$184,839**	**$210,408**	**(23,057)**	**$187,351**

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. Sums may not add to totals due to rounding.

Table 6-12. Performance Measures

Measure	Value (2007$)
Total quantified benefits	$210.4 million
Total quantified costs	$23.1 million
Net present value of net benefits (NPV) (Base year = 1998)	$118.0 million
Benefit-to-cost ratio (BCR)	8.55
Internal rate of return (IRR)	161%

Note: All dollar values were inflation-adjusted to 2007 using the real GDP deflator, chained. NPV was calculated using the 7% real social discount rate recommended by OMB.

7. CONCLUDING REMARKS ON THE EFFECTIVENESS OF THE NCMC CONSORTIUM MODEL

Before NIST's entry into the development of technology infrastructure for combinatorial methods and high-throughput experimentation, the knowledge base was uneven and proprietary. Large chemical firms and their engineering vendors had developed sophisticated solutions for combi using discrete sample libraries, but not for continuous thin films or microfluidics libraries. These firms' knowledge was essentially locked within the silos of corporate research divisions. Given that firms' R&D programs and strategies are a source of competitive advantage, in the absence of a neutral, precompetitive forum, firms had a disincentive to communicate and exchange best practices in combi's development, implementation, and use. This status quo hampered combi's development and uptake as well as a broader awareness of the potential combi holds for increasing throughput and the quantity and quality of data captured per material sample analyzed. A commercial infrastructure for combi for discrete sample libraries based on robotics and automation had emerged, but little technology infrastructure for combi in continuous thin films and microfluidics had emerged.

As a recognized leader in metrology, NIST assumed the role of filling technology gaps left unaddressed because of market and technical barriers. NIST was also able to leverage its reputation for scientific excellence and independence into a leadership role for the technical community. Consequently, benefits from NCMC's novel technologies and of an organization assuming the mantle of leadership of a technical community would not have accrued. The technology NCMC developed between 1998 and 2007 enabled organizations to reap significant R&D efficiency benefits by integrating and adapting for their use methods such as continuous gradient thin films, microfluidics libraries, and the edge lift-off test for interfacial adhesion.

If it were not for these attributes – leadership in metrology, a reputation for scientific excellence, and independence – the creation of a consortium like the NCMC as a precompetitive forum whose members were all from the private sector would have been highly unlikely. Beyond developing and then rapidly transferring technology into the public domain, NCMC's outreach work, research, and publications demonstrated what was possible with combi. Several firms stated that this body of knowledge accelerated their incorporation of combinatorial approaches into their research programs. The publicity and attention NCMC drew to combi made it easier for some researchers to convince senior executives within their organizations to get invest in combinatorial approaches because NCMC and NIST demonstrated that combi for polymers had been successfully performed by a reputable institution.

Through the NCMC's work researchers acquired both technology and evidence of how investments in combi could increase R&D efficiency and hasten the development of more robust polymeric materials and the products whose performance or quality is enabled by those materials. The value generated by the NCMC is evident in the results: firms that adapted NIST's approaches for their needs accrued economic benefits of $165.8 million between 2002 and 2007. Notably, irrespective of whether they adopted any NCMC technology, 50% of survey respondents indicated that NCMC's work accelerated their adoption of combi by an average of 2.3 years. Including benefits from participating in the NCMC ($1.1 million), expanding the combi knowledge base ($24.4 million), and accelerating some firms' combi adoption ($19.0 million), total economic benefits were $210.4 million for the polymeric materials, coatings, and personal care and household products industries. Total costs, inclusive of technology acquisition costs, were $23.1 million, translating into a net economic benefit of $187.4 million. The BCR was 8.55 and the IRR over the analysis period was 161%.

The NCMC offers an exemplary example of much of the best of what NIST has to offer in science & technology development and outreach:

- overcoming technology gaps through the development of infratechnology,
- convening researchers in independent, precompetitive forums to disseminate research and best practice,
- partnering with government and academia to develop and execute research projects of particular relevance to industry,
- demonstrating what is possible and advocating for novel approaches for rapidly identifying research foci, and
- championing the adoption and development of new approaches that offer R&D and production efficiency benefits as well as the opportunity to discover groundbreaking new materials.

The consortium model approved to be particularly effective. The results in Chapter 6 evidence how industry participation in the research program meant that NCMC was developing generic technologies and infratechnologies that responded to infrastructure gaps discovered as industrial research agenda evolved and experience with combi grew. NIST benefited from industry's feedback, and industry benefited from access to information on a prepublication basis as well as from hands-on demonstrations of novel approaches. The feedback loop inherent in this approach balanced NIST's mandate to expand the frontier of measurement science with industry's desire for research outcomes to be relevant to their needs.

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APPENDIX A: LIST OF FIRMS COMPRISING EXTRAPOLATION BASE FOR NATIONAL IMPACT ESTIMATION

- **3M Company**
- Air Products and Chemicals, Inc.
- Albemarle Corporation
- Alberto–Culver Company
- Arch Chemicals, Inc.
- Ashland Inc.
- Avery Dennison Corporation
- Avon Products, Inc.
- BASF SE
- Bayer AG
- Boston Scientific
- BP p.l.c.
- Cabot Corporation
- Celanese Corporation
- Chemtura Corporation
- Church & Dwight Co., Inc.
- Ciba Specialty Chemicals Holding Inc.
- **Colgate–Palmolive Company**
- Cytec Industries Inc.
- E. I. du Pont de Nemours and Company
- Eastman Chemical Company
- Ecolab Inc.
- Elizabeth Arden, Inc.
- Exxon Mobil Corporation
- Ferro Corporation
- FMC Corp
- General Electric Company
- Georgia Gulf Corporation
- H.B. Fuller Company
- Hercules Incorporated
- Hexcel Corporation
- Honeywell International Corp
- Huntsman Corporation
- Illinois Tool Works Inc.
- **Imperial Chemical Industries**
- Intel
- International Flavors & Fragrances Inc.
- Johnson & Johnson
- Kimberly–Clark Corporation
- L'Oréal SA
- LVMH Moët Hennessy Louis Vuitton SA
- New Market Corp
- Nu Skin Enterprises, Inc.
- PolyOne Corporation
- PPG Industries, Inc.
- Praxair, Inc.
- Rayonier Inc.
- Revlon
- Rhodia
- Rockwood Holdings, Inc.
- Rohm and Haas Company
- **RPM International Inc.**
- Sealed Air
- Sensient Technologies Corporation
- Solutia Inc.
- Stepan Company
- The Clorox Company
- The Dow Chemical Company
- The Estée Lauder Companies Inc.
- The Lubrizol Corporation
- The Procter & Gamble Company
- The Sherwin–Williams Company
- The Valspar Corporation
- W. R. Grace & Co.
- Akzo Nobel N.V.
- Arkema
- Michelin Corporation
- Unilever PLC

APPENDIX B: MEMBER SURVEY

Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers

A Survey Sponsored by the National Institute of Standards and Technology (NIST)

Survey Instrument for Current and Former NCMC Members

Combinatorial and high-throughput methods, or “combi,” have been credited with accelerating the pace and quality of polymers R&D within both the private and academic sectors. By enabling material scientists to create large “libraries” of samples and to quickly analyze their properties, combi speeds the discovery of new polymeric materials.

NIST has commissioned RTI International, a not-for-profit research institute, to conduct an evaluation of the adoption of combinatorial methods for organic polymers R&D, the economic impacts associated with this adoption, and the NIST Combinatorial Methods Center (NCMC).

The goals of the study are to:

- learn the extent to which NIST combi technologies have been adopted,
- estimate the impact combi has had on researchers’ productivity, and
- provide guidance on how a NIST-industry consortium model has benefited the technical community.

The following survey is an important effort that seeks to provide insights into the effectiveness of NIST-sponsored, industry-directed programs. Such insights will help shape future strategic directions. The survey is voluntary and is estimated to take between 15 and 20 minutes to complete. It requests:

- estimates of your familiarity with combi and whether you use it,
- when you may have adopted a combinatorial workflow in your lab,
- data on your experience with the NCMC and its work to spur combi’s adoption, and
- measures of how combi may have improved the materials discovery process.

NIST will use the results of this study in its strategic planning for the NCMC, and specifically for its materials science programs. NCMC’s technical contributions to combi for organic polymers have largely been in library fabrication, testing, and analysis of: continuous gradient thin film libraries, discrete libraries, and microfluidics for polymers in organic solvents. Skip questions that are outside your area of expertise.

Responses to this survey will be kept strictly confidential. At no time will any individual’s name, any company or university name, their participation, or identifiable response be released by RTI to any third party, including NIST and the NCMC. The data that survey respondents provide will only be used to present aggregate analytical findings to the NCMC in the form of a final report that will be publicly released by the end of this calendar year following a peer review process.

Questions about the survey should be directed to Dallas Wood at (919) 541-8743 or [US Eastern Time], or Alan O’Connor at (415) 848-1316 or [US Pacific Time].

OMB Control Number 0693-0033, expiration date 7/31/09
This survey is authorized under Executive Order 12862, “Setting Customer Service Standards.” Your response is voluntary and all data collected will be considered confidential. Public reportings for this collection of information is estimated to average 20 minutes per response, including the time of reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this estimate or any other aspects of this collection of information, including suggestions for reducing the length of this questionnaire, to the National Institute of Standards and Technology, 100 Bureau Drive, Stop 3220, Gaithersburg, MD, 20899-3220 and the Office of Management and Budget Information and Regulatory Affairs, Office of Management and Budget, Washington, DC 20503.

1. Respondent Contact Information

Responses to this survey are strictly confidential. At no time will any individual's name, any company name, participation, or identifiable response be released by RTI to any third party, including the NIST and the NCMC.

Respondent name (optional):

Affiliation (optional):

Title (optional):

Telephone number (optional)

Email (optional):

Geographic location, if not USA:

Are you willing to participate in a short, confidential follow-up telephone discussion about your response? **[Select One]**

2. Combinatorial and/or High Throughput Methods ("Combi") Usage.

Does your company or university research laboratory (-ies) currently use any combinatorial or high-throughput methods (referred to as "combi") for polymers R&D, or has it used combi in the past?

☐ Yes, we are currently using combi in my lab.

Approximately how many years has combi been used in your lab?

Did your company join the NCMC as part of a combi adoption plan?

☐ No, we are not using combi in my lab.

If no, do you expect to use combi in the future?

did your lab suspend using combi?

Comments?

3. Combi Technology Adoption Timeframe.

The following questions ask about your lab's adoption of combi for polymers R&D. Our goal is to track the diffusion of the combi technology and methods. Please answer the following questions to the best of your ability. Your best approximation will suffice.

3a. In which year(s) would you estimate that the following occurred?

Researchers in our lab became aware of the successful, **practical use** of combi for polymers R&D

My lab(s) implemented and began using combi for the first time

Combi became a part of the regularly used methods in our lab(s)

Comments?

3b. Reflect upon your familiarity with the NCMC's papers, workshops, proceedings, and/or conference presentations. Did the research offered at conferences or in the technical literature accelerate your lab's adoption of combi overall?

☐ Yes, this research likely accelerated our adoption of combi by years.

☐ No, this research likely had little impact on the timing of our combi adoption.

4. Laboratory Personnel Working in Combi.

The purpose of this section is to estimate how many researchers may be using combi for R&D and how that estimate changed over time. This information will be combined with other responses to estimate the number of people working in combi today. If you are unsure of an estimate for any given year, simply leave the cell empty.

4a. Approximately how many full-time equivalent employees (FTEs) worked in combi in your lab during the following years? Please separate those FTEs that were primarily involved in developing/adopting/adapting new combi methods from those FTEs that were primarily involved in the regular use of established combi methods.

Year	**1999**	**2001**	**2003**	**2005**	**2007**
FTE(s) primarily involved in developing/adopting/adapting new combi methods					
FTE(s) primarily involved in regular use of established combi methods					

4b. What percent of your combi activity currently falls within each of the following library types?

	2003	Current
Thin films libraries	**%**	**%**
Discrete libraries	**%**	**%**
Microfluidics libraries	**%**	**%**

Comments?

5. Technology Adoption of Combi Methods and Technologies.

5a. What magnitude of labor productivity increase (tests per day per researcher) do you estimate that **combi in general** offers your lab overall? **[Select One]**

5b. Please indicate whether you use or adapted any of the following methods and technologies developed by the NCMC and its industry members.

	Use or adapted this technology	Aware of, but not relevant to your research	Unaware of this technology
Continuous thin films with gradients in temperature, composition, thickness, surface energy, or on chemically patterned substrates	☐	☐	☐
Discrete libraries used with gradients in temperature, surface energy, or thickness	☐	☐	☐
Microfluidics produced organic solvent-based libraries	☐	☐	☐
Buckling method of modulus measurement for thin films and soft materials	☐	☐	☐
Edge lift-off test for interfacial adhesion	☐	☐	☐
Multi lens contact test for adhesion	☐	☐	☐
Interfacial tension measurement via microfluidics	☐	☐	☐
High throughput measurement of morphology	☐	☐	☐
Integrated metrology (morphology, composition, extent of reaction) on microfluidics produced organic solvent-based libraries	☐	☐	☐

5c. If you use or adapted any of the NCMC technologies listed in 5b, did they offer efficiency benefits or cost savings over what your lab had been using heretofore? **[Select One]**

If yes, please estimate the combined benefits adoption of these NCMC technologies had on the following factors:

Increase in research labor productivity: (tests per day per researcher)	**[Select One]**
Reduced materials expenses, per 10 samples processed:	**US$**
Savings on research equipment expenditures (excluding one-time adoption costs):	**US$**
Time Savings:	**[Select One]**

Comments?

5d. Did the NCMC technologies you adopted or adapted from 5b improve the quality of your research or any products that your company may produce? **[Select One]**

Comments?

5e. Did the NCMC technologies you adopted or adapted from 5b enable you to test samples over a broader range of conditions? **[Select One]**

5f. Please estimate the one-time costs you incurred when adopting or adapting any of the NCMC technologies listed in Question 5b. Would you characterize these expenses as a large investment in labor, research equipment, or instillation relative to other technologies your lab has adopted?

Comments:

6. Benefits of Consortium Membership.

The following questions ask you to reflect upon the economic benefits your organization accrues from participating in the NCMC.

6a. Did participation in the NCMC offer more productive marketing or networking opportunities, relative to other conferences or combi meetings? **[Select One]**

If yes, how would you rank the productivity of these NCMC meetings relative to other conferences or combi meetings?

Not Much More Productive	Slightly More Productive	Significantly More Productive
☐	☐	☐

6b. Did participation in the NCMC validate or invalidate internal research projects and permit more efficient and effective resource allocation? **[Select One]**

Did participation in the NCMC help your organization avoid any research activities, or enable your organization to acquire needed research more quickly or cost effectively? **[Select One]**

If yes, please estimate the costs your firm likely saved and the amount of time

Labor (in FTEs or person-months):	**[Select One]**
Materials Expense	US$
Research equipment	US$
Time	**[Select One]**

Over what time period did you accrue these benefits:

6c.	Did the NCMC offer valuable researcher training and demonstrations beyond what would have been available elsewhere?	**[Select One]**
	If yes, approximately how many training hours were likely saved, per meeting, had researchers attempted to acquire the same amount and quality of research via readings and/or conference attendance?	hours
6d.	Was the annual benefit your organization accrued from participation in the NCMC greater than, equal to, or less than the annual membership fees it paid?	**[Select One]**
6e.	If you would like to offer comments about the NCMC, its effectiveness and usefulness consortium, or offer suggestions for its improvement or expansion, please do so below.	
	Comments:	

APPENDIX C: NONMEMBER SURVEY

Economic Impacts from the Adoption of Combinatorial Methods for Organic Polymers

A Survey Sponsored by the National Institute of Standards and Technology (NIST)

Combinatorial and high-throughput methods, or "combi," have been credited with accelerating the pace and quality of polymers R&D within both the private and academic sectors. By enabling material scientists to create large "libraries" of samples and to quickly analyze their properties, combi speeds the discovery of new polymeric materials.

NIST has commissioned RTI International, a not-for-profit research institute, to conduct an evaluation of the adoption of combinatorial methods for organic polymers R&D, the economic impacts associated with this adoption, and the NIST Combinatorial Methods Center (NCMC). Respondents do not need to be using combi in order to participate.

The goals of the study are to:

- learn the extent to which NIST combi technologies have been adopted,
- estimate the impact combi has had on researchers' productivity, and
- provide guidance on how a NIST-industry consortium model has benefited the technical community.

The following survey is an important effort that seeks to provide insights into the effectiveness of NIST-sponsored, industry-directed programs. Such insights will help shape future strategic directions. The survey is voluntary and is estimated to take between 15 and 20 minutes to complete. It requests:

- estimates of your familiarity with combi and whether you use it,
- when you may have adopted a combinatorial workflow in your lab,
- information on your familiarity with the NCMC and its work to spur combi's adoption, and
- measures of how combi may have improved the materials discovery process.

NIST will use the results of this study in its strategic planning for the NCMC, and specifically for its materials science programs. NCMC's technical contributions to combi for organic polymers have largely been in library fabrication, testing, and analysis of continuous gradient thin film libraries, discrete libraries, and microfluidics for polymers in organic solvents. Skip questions which are outside your area of expertise.

Responses to this survey will be kept strictly confidential. At no time will any individual's name, any company or university name, their participation, or identifiable response be released by RTI to any third party, including NIST and the NCMC. The data that survey respondents provide will only be used to present aggregate analytical findings to the NCMC in the form of a final report that will be publicly released by the end of this calendar year following a peer review process.

Questions about the survey should be directed to Dallas Wood at (919) 541-8743 or [US Eastern Time], or Alan O'Connor at (415) 848-1316 or [US Pacific Time].

OMB Control Number 0693-0033, expiration date 7/31/09
This survey is authorized under Executive Order 12862, "Setting Customer Service Standards." Your response is voluntary and all data collected will be considered confidential. Public reportings for this collection of information is estimated to average 20 minutes per response, including the time of reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this estimate or any other aspects of this collection of information, including suggestions for reducing the length of this questionnaire, to the National Institute of Standards and Technology, 100 Bureau Drive, Stop 3220, Gaithersburg, MD, 20899-3220 and the Office of Management and Budget Information and Regulatory Affairs, Office of Management and Budget, Washington, DC 20503.

1. Combinatorial and/or High Throughput Methods (“Combi”) Usage.

Does your company or university research laboratory (-ies) currently use any combinatorial or high-throughput methods (referred to as “combi”) for polymers R&D, or has it used combi in the past?

☐ Yes, we are currently using combi in my lab.

☐ I do not know if we are using combi.

☐ No, we are not using combi in my lab.

If yes, approximately how many years has combi been used in your lab?

If no, do you expect to use combi in the future?

did your lab suspend using combi?

Comments? ____________________

2. Combi Technology Adoption Timeframe.

The following questions ask about your lab’s adoption of combi for polymers R&D. Our goal is to track the diffusion of the combi technology and methods. Please answer the following questions to the best of your ability. <u>Your best approximation will suffice.</u>

2a. In which year(s) would you estimate that the following occurred?

Researchers in our lab became aware of the successful, **practical use** of combi for polymers R&D

My lab(s) implemented and began using combi for the first time

Combi became a part of the regularly used methods in our lab(s)

Comments? ____________________

2b. Are you familiar with the NIST Combinatorial Methods Center (NCMC), a NIST-sponsored research consortium that works with industry members to advance the combi technology, measurement, and analysis needs (http://polymers.msel.nist.gov/combi/index.html)?

☐ No, I am not familiar with the NCMC.

☐ Yes, I am familiar with or have heard of the NCMC.

How did you hear about the NCMC? Please select all that apply.

- ☐ Conferences, seminars, or workshops
- ☐ Technical literature
- ☐ Trade journal article(s)
- ☐ Word of mouth
- ☐ Other (please specify):____________________

2c. The NCMC made several presentations and sponsored symposia about combi at recent conferences. Have you attended any of the following meetings or conferences since 2001?

☐ American Chemical Society	☐ American Physical Society
☐ Materials Research Society	☐ Knowledge Foundation Conferences
☐ Gordon Conferences	☐ Intl Workshop on Combinatorial Materials Science
☐ NCMC Industry Workshops	☐ Other:

☐ I did not attend any of the above conferences or workshops.

2d. The NCMC published its research in the technical literature to support academic and industry researchers in their adoption of combi. Authors included E.J. Amis, A. Karim, J.C. Meredith, C.M. Stafford, M.J. Fasolka, and K.L. Beers, among others. Are you familiar with the research of these authors?

☐ Yes, I am familiar with one or more of the above authors’ research.

☐ No, I am not familiar with any of the above authors' research.

2e. Reflect upon your familiarity with the NCMC's papers and/or conference presentations. Did the research offered at conferences or in the technical literature accelerate your lab's adoption of combi overall?

☐ Yes, this research likely accelerated our adoption of combi by years.

☐ No, this research likely had little impact on the timing of our combi adoption.

3. Technology Adoption of Combi Methods and Technologies.

3a. What magnitude of labor productivity increase (tests per day per researcher) do you estimate that **combi in general** offers your lab overall? **[Select One]**

3b. Please indicate whether you use or adapted any of the following methods and technologies developed by the NCMC and its industry members.

	Use or adapted this technology	Aware of, but not relevant to your research	Unaware of this technology
Continuous thin films with gradients in temperature, composition, thickness, surface energy, or on chemically patterned substrates	☐	☐	☐
Discrete libraries used with gradients in temperature, surface energy, or thickness	☐	☐	☐
Microfluidics produced organic solvent-based libraries	☐	☐	☐
Buckling method of modulus measurement for thin films and soft materials	☐	☐	☐
Edge lift-off test for interfacial adhesion	☐	☐	☐
Multi lens contact test for adhesion	☐	☐	☐
Interfacial tension measurement via microfluidics	☐	☐	☐
High throughput measurement of morphology	☐	☐	☐
Integrated metrology (morphology, composition, extent of reaction) on microfluidics produced organic solvent-based libraries	☐	☐	☐

3c. If you use or adapted any of the NCMC technologies listed in the previous question, did they offer efficiency benefits or cost savings over what your lab had been using heretofore? **[Select One]**

If yes, please estimate the combined benefits adoption of these NCMC technologies had on the following factors:

Increase in research labor productivity:	**[Select One]**
Reduced materials expenses, per 10 samples processed:	**US$**
Savings on research equipment expenditures (excluding one-time adoption costs):	**US$**
Time Savings:	**[Select One]**

Comments?

3d. Did the NCMC technologies you adopted or adapted (from 3b) improve the quality of your research or any products that your company may produce? **[Select One]**

Comments?

3e. Did the NCMC technologies from 3b enable you to test samples over a broader range of conditions? **[Select One]**

3f. Please estimate the one-time costs you incurred when adopting or adapting any of the NCMC technologies listed in Question 3b. Would you characterize these expenses as a large investment in labor, research equipment, or instillation relative to other technologies your lab has adopted?

Comments:

4. Laboratory Personnel Working in Combi.

The purpose of this section is to estimate how many researchers may be using combi for R&D and how that estimate changed over time. This information will be combined with other responses to estimate the number of people working in combi today. If you are unsure of an estimate for any given year, simply leave the cell empty.

4a. Approximately how many full-time equivalent employees (FTEs) worked in combi in your lab during the following years? Please separate those FTEs that were primarily involved in developing/adopting/adapting new combi methods from those FTEs that were primarily involved in the regular use of established combi methods.

Year	1999	2001	2003	2005	2007
FTE(s) primarily involved in developing/adopting/adapting new combi methods					
FTE(s) primarily involved in regular use of established combi methods					

4b. What percent of your combi activity currently falls within each of the following library types currently and in 2003?

	2003	Current
Thin films libraries	%	%
Discrete libraries	%	%
Microfluidics libraries	%	%

Comments:

5. Organization or Industry Classification.

Please indicate which of the following best describes your lab.

☐ Advanced materials lab (e.g. resins, synthetic rubbers, artificial synthetic fibers)
☐ Coatings, adhesives, paints, and pigments lab
☐ Personal care and household products lab
☐ University research laboratory
☐ Government or institutional research laboratory
☐ Other:

6. Activity and Size Measures.

RTI has obtained industry-level measures of economic activity, and would like to aggregate your responses with those of others to extrapolate to industry-level measures. The measures below will <u>only</u> be used to combine your responses with those of others. Again, your best approximation will suffice.

6a. For private-sector respondents:

Stock trading symbol ("Ticker"):

Approximate 2007 company sales revenue: **million US$**

Approximate 2007 company R&D expenditures: **million US$**

6b. For academic and public sector respondents:

Approximate 2007 laboratory or department funding: **million US$**

Approximate 2007 full-time equivalent staffing: **FTEs**

Approximate number of student staff (all levels): **students**

7. Respondent Contact Information

Responses to this survey are strictly confidential. At no time will any individual's name, any company name, participation, or identifiable response be released by RTI to any third party, including the NIST and the NCMC.

Geographic location, if not USA: ______________________________

Respondent name (optional): ______________________________

Affiliation (optional): ______________________________

Title (optional): ______________________________

Telephone number (optional) ______________________________

Email (optional): ______________________________

Are you willing to participate in a short, confidential follow-up telephone discussion about your response? If so, please ensure that you provided your email address or telephone number above. **[Select One]**