An Assessment of the National Institute of Standards and Technology Chemical Science and Technology Laboratory: Fiscal Year 2009

Panel on Chemical Science and Technology; National Research Council

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This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

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Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations, nor did they see the final draft of the report before its release. The review of this report was overseen by Alton D. Slay, Warrenton, Virginia. Appointed by the National Research Council, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the authoring panel and the institution.

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Summary

Overall, the Chemical Science and Technology Laboratory (CSTL) of the National Institute of Standards and Technology (NIST) is meeting its obligations, objectives, and desired impacts, and its priorities are appropriate and aligned with NIST's mission and priorities. The technical merit of the laboratory and the commitment of the staff are high. There is no evidence that any programs are jeopardized by a lack of facilities or equipment, and ongoing and planned new facility construction should greatly improve CSTL capabilities. The National Research Council's Panel on Chemical Science and Technology has the following comments about the operation of the laboratory within this framework of CSTL's clear and consistent success and high technical merit.

1. The panel highlights the importance of having a CSTL strategic plan, involving all divisions and geographical locations, including a roadmap for progress, and commends the CSTL's efforts in developing one.
2. It is important for the CSTL to have a methodology and program for evaluating projects with respect to their contribution to the CSTL and NIST missions. This approach will facilitate the elimination of programs when they are no longer effective in meeting desired goals. The project prioritization process adopted by the CSTL is a positive step, and the panel looks forward to the execution of the process.
3. Because of stable core funding, the CSTL does well with long-term programs that are aligned with the NIST mission.
4. Greater external visibility of the professional staff and their nomination for external awards should be emphasized more; a committee to nominate staff for external awards would help in this regard.
5. The CSTL should continue to emphasize the importance of its staff publishing in high-impact, refereed journals and giving invited talks. If these factors are to be used as performance standards and metrics, they and all other standards and metrics should be clearly communicated to the staff.
6. Information technology problems related to system shutdowns and independent database development within CSTL divisions should be addressed. A policy change at the NIST level is required.
7. Biological topics are becoming an increasing theme at the CSTL and NIST levels. The following are factors that the CSTL should consider in going forward:
   A. How will the CSTL prioritize the participation of the divisions, especially with respect to hiring decisions?
   B. What is the leadership role of the Biochemical Science Division?
   C. How will the CSTL coordinate its activities throughout its divisions and with other laboratories in NIST?
   D. How will the CSTL strategically partner with agencies and institutions outside NIST? How will workshops be a part of this partnering?
   E. Measurements and standards are NIST's niche in this area.

8. With respect to intellectual property, a consistent policy on disclosures, copyrighting, and marketing is needed at the NIST level; this policy must be disseminated throughout the organization.
9. Joint appointments of professional staff to two separate divisions within the CSTL would provide more flexibility in adding personnel in high-priority areas and would enhance interdisciplinary activities. Joint appointments with institutions outside NIST would also add to interdisciplinary capabilities.
10. The CSTL should examine the balance of technicians versus PhD scientists to ensure that the scientists' time is used most productively and efficiently. The addition of a few technicians might greatly improve the productivity and efficiency of the entire technical staff.
11. The Process Measurements Division has been successful in automating its Thermometry Laboratory, with impressive results. This effort could serve as a model for automating other measurement laboratories that conduct repetitive tasks which must be done in a particular way.
12. The CSTL should continue to seek, and should act on opportunities to lead in, collaborative activities in areas where it has strong expertise and where it has equipment available for use.
13. The CSTL should consider and investigate media opportunities to publicize the usefulness of its capabilities. The panel thinks that more potential users of NIST services and products would come forward if they knew more about what NIST has to offer.

1

The Charge to the Panel and the Assessment Process

At the request of the National Institute of Standards and Technology (NIST), the National Research Council (NRC) has since 1959 annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering environments to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now nine,[1] as well as the adequacy of the laboratories' resources. In 2009, NIST requested that five of its laboratories be assessed: the Center for Nanoscale Science and Technology, the Chemical Science and Technology Laboratory (CSTL), the Electronics and Electrical Engineering Laboratory, the Information Technology Laboratory, and the NIST Center for Neutron Research. Each of these was assessed by a separate panel of experts; the findings of the respective panels are summarized in separate reports. This report summarizes the findings of the Panel on Chemical Science and Technology.

For the fiscal year (FY) 2009 assessment, NIST requested that the panel consider the following criteria as part of its assessment:

1. The technical merit of the current laboratory programs relative to current state-of-the-art programs worldwide;
2. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and
3. The degree to which laboratory programs in measurement science and standards achieve their stated objectives and desired impact.

The context of this technical assessment is the mission of NIST, which is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve the quality of life. The NIST laboratories conduct research to anticipate future metrology and standards needs, to enable new scientific and technological advances, and to improve and refine existing measurement methods and services.

In order to accomplish the assessment, the NRC assembled a panel of 21 volunteers, whose expertise matches that of the work performed by the CSTL staff.[2] The panel members were also assigned to six subgroups (division review teams), whose expertise matched that of the work performed in the six divisions in the CSTL: Analytical Chemistry, Biochemical Science, Chemical and Biochemical Reference Data, Process Measurements, Surface and Microanalysis Science, and Thermophysical Properties. These division review teams (each led by a team leader chosen from within the panel) individually visited the CSTL facilities in Gaithersburg, Maryland, and Boulder, Colorado, for 1 or 2 days, during which time they

[1]The nine NIST laboratories are the Building and Fire Research Laboratory, the Center for Nanoscale Science and Technology, the Chemical Science and Technology Laboratory, the Electronics and Electrical Engineering Laboratory, the Information Technology Laboratory, the Manufacturing Engineering Laboratory, the Materials Science and Engineering Laboratory, the NIST Center for Neutron Research, and the Physics Laboratory.

[2] See http://www.cstl.nist.gov/ for more information on CSTL programs. Accessed June 1, 2009.

attended presentations, tours, demonstrations, and interactive sessions with CSTL staff. Subsequently, the entire panel assembled for 2 days at the Hollings Marine Laboratory in Charleston, South Carolina. There they toured the laboratory and attended overview presentations by CSTL management and interactive sessions with CSTL managers. The panel also met at this time in a closed session to deliberate on its findings and to define the contents of this assessment report.

The approach of the panel to the assessment relied on the experience, technical knowledge, and expertise of its members, whose backgrounds were carefully matched to the technical areas of CSTL activities. The panel reviewed selected examples of the technological research covered by the CSTL; because of time constraints, it was not possible to review the CSTL programs and projects exhaustively. The examples reviewed by the panel were selected by the CSTL. The panel's goal was to identify and report salient examples of accomplishments and opportunities for further improvement with respect to the following: the technical merit of the CSTL work, its perceived relevance to NIST's own definition of its mission in support of national priorities, and specific elements of the CSTL's resource infrastructure that are intended to support the technical work. These examples are intended collectively to portray an overall impression of the laboratory, while preserving useful suggestions specific to projects and programs that the panel examined. The assessment is currently scheduled to be repeated biennially, which will allow, over time, exposure to the broad spectrum of CSTL activity. While the panel applied a largely qualitative rather than a quantitative approach to the assessment, it is possible that future assessments will be informed by further consideration of various analytical methods that can be applied.

The comments in this report are not intended to address each program within the CSTL exhaustively. Instead, this report identifies key issues. Given the necessarily nonexhaustive nature of the review process, the omission of any particular CSTL program or project should not be interpreted as a negative reflection on the omitted program or project.

The rest of this report is organized in six chapters, which provide a detailed discussion of the assessment of the individual CSTL divisions, including resulting recommendations.

2

Analytical Chemistry Division

OVERVIEW

The activities of the Analytical Chemistry Division (ACD) of the Chemical Science and Technology Laboratory are focused primarily in two areas—fundamental chemical metrology and the development of measurement methods and standards, including the following: clinical diagnostics and health status markers, environmental monitoring, food dietary supplements and nutritional assessment, industrial commodities and advanced materials characterization, forensics and homeland security, nanoparticle characterization, and the hydrogen economy. The division maintains core expertise in analytical mass spectrometry, analytical separation science, atomic and x-ray fluorescence spectrometry, gas metrology, nuclear analytical methods, nuclear magnetic resonance (NMR) spectrometry, and classical and electroanalytical chemistry. The core expertise resides in four groups or teams (Organic Chemical Metrology Group, Inorganic Chemical Metrology Group, Gas Metrology Group, and Environmental Specimen Bank/NMR Team) and provides the capability for carrying out the division's broad mission with flexibility so that it can respond to changing and evolving national priorities. The Environmental Specimen Bank/NMR Team is located at the Hollings Marine Laboratory (HML) in Charleston, South Carolina, which is a partnership with the National Oceanic and Atmospheric Administration (NOAA), the South Carolina Department of Natural Resources, the Medical University of South Carolina, and the College of Charleston.

The total FY 2008 ACD funding was $21.82 million, of which $4.23 million (19 percent) was other-agency funding and $5.29 million (24 percent) was from standard reference materials (SRMs). As of March 2009, total funding was $21.29 million (including $0.39 million pending), of which $3.89 million (including $0.23 million pending), or 18 percent, was other-agency funding and $4.22 million (20 percent) was from SMRs. The division staffing level is approximately 90 NIST full-time equivalents (FTEs) and 15 visiting scientists and graduate students.

The ACD has been meeting its obligations, and its priorities are appropriate. The technical commitment of the staff is high, and the availability of equipment and facilities is generally of a high order. The strong tradition of quantitative measurements within the ACD is very important work that helps many federal and state agencies achieve their goals. Examples include the division's support of the Consumer Product Safety Improvement Act of 2008 (Public Law 110-314), which addressed the need to detect lead (Pb) in paint on children's toys; its assistance to the Environmental Protection Agency (EPA) in its mission to regulate mercury (Hg) in emissions from coal-powered-electricity generation; and its development of standards for the Office of Dietary Supplements in the National Institutes of Health (NIH).

RESPONSE TO RECOMMENDATIONS FROM THE PREVIOUS REPORT

One of the concerns expressed by the Panel on Chemical Science and Technology during its 2007 review[1] centered on the general balance between service work and methods research. The concern is now formulated more precisely, as follows: the development of standard reference materials (SRMs) is a key component of the work of the ACD, and balance is needed between developing SRMs and establishing new analysis methods. The division does an excellent job of developing assays for the quantitative analysis of target analytes in a broad range of matrices—an area in which it excels. However, the panel raised concerns during its 2007 review about a shortage of staff in aerosol science and electrochemistry (listed among the ACD's areas of core expertise), and those concerns remain unaddressed, as noted elsewhere in this chapter.

TECHNICAL MERIT

In 2007, division researchers produced 57 publications and gave 163 talks (64 invited). In 2008, division researchers produced 66 publications and gave 162 talks (71 invited). For 2007–March 2009, 8 external awards and 7 internal awards were given to ACD staff.

Projects Within the Organic Chemical Metrology Group

The Organic Chemical Metrology Group has a long history of excellence in quantitative measurements, particularly in separations. The group has diversified more recently into proteomics, NMR, and other techniques and is applying these techniques to important areas, such as nutritional analysis and marine environmental samples. Standards for conducting quantitative measurements of proteins are not well developed across the community, and the work being done by this project is both timely and important. The linkage of the project with leading proteomics projects through the National Cancer Institute (NCI) Clinical Proteomics Technology Assessment for Cancer (CPTAC) collaboration is especially valuable and connects the ACD staff with strong researchers in the field. Given the number of laboratories now engaged in proteomics, many of which do not have resident mass spectrometry experts, having standards for assessing the operation of the instrument and quality of the results is very important. These results are also being published in significant journals by members of the group as coauthors. However, this group should be leading publications in this area. Furthermore, it should consider the addition of a protein mass spectrometrist and a high-performance mass spectrometer to support its continuing work in proteomics and metabolomics. This group reported that it is expressing its own labeled proteins; it may want to consider working with other projects that do this on a large scale (e.g., structural biology projects), and it would have the infrastructure to do this. The metabolomics work, like the proteomics work, is very important; this project has been using multiple approaches to develop techniques and evaluate standards.

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[1] National Research Council, *An Assessment of the National Institute of Standards and Technology Chemical Science and Technology Laboratory: Fiscal Year 2007.* Washington, D.C.: The National Academies Press, 2007.

The Analytical Chemistry Division is well known for its fundamental studies on shape recognition using reversed-phase chromatography. Strong progress on these efforts continues, with detailed molecular modeling studies on the three-dimensional structural attributes of these stationary phases. Based on this work and on its recent study on the solvation of perfluorinated octane, the division is now examining new stationary phases that utilize perfluoro functionalities; this should allow even greater molecular recognition.

The work on establishing standards for nutritional analysis has very high importance, and it provides good support for other federal agencies and in the arena of public health. A large number of SRMs have been developed—a need that will grow in the future. In addition to standards for nutritional supplement labeling, standards are being established for botanical supplements. This area is also growing quickly, and reliable methods for analyzing these supplements are very important. The development of techniques for the analysis of contaminants in human biofluids builds on long-standing expertise in understanding the impact of matrices on various assays.

The forensics and homeland security project, which interacts closely with the Department of Homeland Security (DHS) on the development of SRMs for the analysis of explosives, is one of several such efforts at NIST. The project has developed trace-explosive SRMs for use in portable instruments that are a vast improvement on the use of standards provided by manufacturers. The forensics and homeland security project has also begun to develop metrology and standards for canine detection of trace explosives. It was unclear whether the ACD group's project has developed sufficient interactions with other groups outside of NIST with relevant experience. For example, the ACD will need to develop increased interaction with a larger project of forensics researchers if it is to optimize its participation in any NIST-wide response to the recent National Research Council report on forensics science.[2]

Projects Within the Inorganic Chemical Metrology Group

The Inorganic Chemical Metrology Group (ICMG) shows excellence in a range of analysis techniques, including inductively coupled plasma mass spectrometry (ICP-MS), inductively coupled plasma optical emission spectrometry (ICP-OES), neutron imaging, and x-ray fluorescence (XRF) spectrometry. The neutron imaging activities are aimed at achieving high-resolution (submicron) imaging. Neutron imaging has the potential to provide a quantum leap for materials research in fuel cell dynamics and hydrogen storage; for biological research, such as in nanomedicine; and for environmental research, including that on global warming. Major accomplishments of this innovative group include the development of new neutron converter prototypes and interesting designs of radiography components.

A very important ICMG study examines tissue-banked samples of seabird eggs from different locations in and around Alaska. An important set of new high-precision isotopic reference materials (RMs) containing multiple elements is being developed. Four new isotopic RMs containing Hg, Pb, thallium (Tl), and germanium (Ge) are planned for 2009-2010 that will provide an important high-precision reference material for the community. This work was enabled by the acquisition of an inductively coupled plasma multicollector mass spectrometer with precision of a few parts in 10^6.

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[2] National Research Council, *Strengthening Forensic Science in the United States: A Path Forward*. Washington, D.C.: The National Academies Press, 2009.

Quantification of deoxyribonucleic acid (DNA) at the trace and ultratrace levels is of increasing importance in bioanalysis connected to applications such as nanoparticle drug delivery and disease monitoring. The ICMG is using ICP-OES to monitor the phosphorus emission signal from DNA. Plans to move to high-resolution ICP-MS from this project are a productive extension of this research project.

Handheld XRF devices have been manufactured to determine whether lead is present in the paint on imported toys. SRMs are needed to support these screening assays for low levels of lead. ICMG staff are developing new SRMs for this purpose and are benchmarking the new handheld instruments to determine if they can actually meet the performance standards of the Consumer Product Improvement Act of 2008.

This group has also developed a number of new standard reference materials since the panel's 2007 review. Those of significant interest include the newly collected soil sample polluted with 500 parts per million (ppm) hexavalent chromium, the renewal of the San Joaquin soil, and urban dust.

The use of nanoparticles in medical and other applications continues to increase, and the ICMG has been working to establish capabilities for analyzing nanomaterials such as gadolinium-based magnetic resonance imaging (MRI) contrast agents, carbon nanotubes, and gold (Au) nanoparticles. One study on separating free and ligated-gadolinium-based MRI contrast agents is an important effort. However, this effort may not be at the leading edge of this technology, and more interaction with leaders in this area would be valuable to the project. The project on the development of a carbon nanotube SRM in collaboration with national laboratories in Canada demonstrated good scientific rigor. Ultimately, the impact of this standard will require the NCI and other health regulatory bodies to adopt it as a standard for carbon nanotube toxicity tests. The work on ICP-MS of Au nanoparticles and argon (Ar) gas electrospray ionization explores important scientific issues and is interesting; nevertheless, this work might benefit from interaction with a broader array of outside experts in these areas.

Inorganic electrochemistry is a capability that is missing in this group. Because this area is central to both the hydrogen economy and growing research and development activity in battery technologies, there is a clear need to hire a new PhD-level electrochemist, as was noted in the panel's 2007 review.

Projects Within the Gas Metrology Group

The Gas Metrology Group is fulfilling the current standardization needs of several industrial and federal regulatory communities. It provides gas standards that will be required for monitoring all of the established greenhouse gases. This group is also well prepared to move into the realm of gases likely to come under regulation in future years, such as the halocarbons. The project effectively plays a central role among the national metrology institutes (NMIs) on various aspects of monitoring global warming gases. The project is also preparing the laboratory and SRM infrastructure needed for the hydrogen economy.

The Gas Metrology Group's close interaction with the Environmental Protection Agency and instrument manufacturers will soon complete scientifically sound and legally defensible protocols for monitoring Hg emissions from coal-fired electricity generation plants. These efforts have been critical to the Mercury Demonstration Project and the EPA's mandate to regulate Hg emission from coal combustion, which constitutes a major national environmental problem as the dominant anthropogenic source of environmental Hg contamination.

Related standards projects support important international atmospheric monitoring activities such as the World Metrology Organization's Global Atmosphere Watch Program. For example, the NIST Standard Reference Photometer is critical to ozone measurement traceability.

The addition of two permanent BSc-level scientists to this unit since 2007 has improved the ability to support the activities of the Gas Metrology Group. However, there remain two significant, looming shortcomings in this group. The first is one of succession—the project has not yet recruited any new PhD-level permanent staff scientists needed to ensure continuity in this project in the coming decades. This short-staffing could quickly become dire if cap-and-trade schemes for controlling global warming gas emissions are mandated nationally. The second shortcoming is the absence of expertise in the area of atmospheric aerosols, which arguably account for the largest uncertainty in models of global warming and are the subject of increasing activity by the scientific community. As opportunities in this area quickly develop, the ACD should strategically evaluate the direction of this group and the recruiting strategies required to ensure the group's future success. For example, the division should consider adding scientists experienced in aerosol mass spectrometry and high-resolution gas phase spectroscopy, among other areas.

SUMMARY

The Analytical Chemistry Division continues its high-impact contributions in key areas of importance to industry, federal agencies, and researchers across the nation and around the world. The staff's work is well aligned with NIST's core missions. Over the years, the ACD has evolved from instrumentation research to focusing more on establishing standards and analytical methodologies. This is a reflection of the field in analytical chemistry in general. The division must continue to implement and evaluate state-of-the-art technology in analytical chemistry. It also needs to maintain awareness of new developments in the field so that it can adapt quickly to new techniques as well as develop them in-house. The ACD has been reaching out to collaborate with many research groups, both inside and outside NIST. With its valuable expertise, the ACD should take action to be leading more of these collaborations.

Cutting-edge work with potentially high impact is highly evident within the ACD, including the neutron imaging work and the Hg isotope ratio work on marine tissue. The division is doing an excellent job of generating standards and trace analysis methodologies using commercial instrumentation, which is congruent with its mission. In a few areas, the methods being used may not be leading-edge.

The ACD has highly recognized strengths, yet it must be careful that over the long term it does not evolve to having primary expertise in its currently strong areas of separation science and inorganic analysis. Maintaining new perspectives is critical for the division's future. ACD management should reinforce hiring practices that bring in new people with new perspectives, including perspectives that result from training in other organizations. Having the division's young environmental scientist from Charleston, South Carolina, receive further training in France is a good example of broadening perspectives by bringing in people with multidisciplinary backgrounds.

An important aspect of this division's output is its reporting of results to the scientific community. At present, the rate is about one publication per scientific FTE. It is recommended that the ACD work with its staff to increase its publication rate, with more publications in high-impact journals such as *Analytical Chemistry, Nature Methods,* and others, where the work of the division would be read by a broader audience of the analytical chemistry community. In addition, more attention should be given to having ACD staff become more visible in the scientific community.

3

Biochemical Science Division

INTRODUCTION

The Biochemical Science Division (BSD) has the charge of biochemically and biologically based measurement methods, data, reference materials, and predictive models. It has a diverse staff that includes 56 scientists and 45 guest researchers. The division is structured as six research groups: Cell Systems Science, Applied Genetics, Macromolecular Structure and Function, Multiplexed Biomolecular Science, Bioassay Methods, and DNA Science. There are four cross-boundary teams: Nanotoxicity, Microfluidics, Biosecurity, and Cellular Biometrology. As described below, the panel reviewed the six research groups and one of the cross-boundary teams (Nanotoxicity) as an example of how the team concept functions.

The BSD budget is derived primarily from the scientific and technical research services (STRS) funding (68 percent). Mission-focused research from other agencies contributes 22 percent to the budget. The division also generates approximately $0.8 million annually from measurement services. Sixty-five percent of the budget is invested in bioscience and health-related activities. The BSD also receives approximately $500,000 per year to purchase capital equipment.

In addition to the broad assessment criteria described in Chapter 1, the panel considered the following issues in its assessment of the Biochemical Science Division:

1. What are the unique contributions made by the division that result from its being at NIST?
2. Does work in the division result in a NIST product?
3. Is the division operating at a state-of-the-art level in each of its component groups?
4. Is the division greater than the sum of its parts?

TECHNICAL MERIT

Overall, the reorganization of the Biochemical Science Division over the past 2 years has produced positive outcomes. The division has been restructured into six groups, each with a group leader. Cohesion within the division has been addressed by establishing crosscutting technology teams. These teams were not well defined; how they function was not made clear to the panel. One of these intramural teams, the Nanotoxicity Team, served as a sample to provide insights into how this concept functions. The Nanotoxicity Team was very enthusiastic, but the strategy for technical management of the team was not made clear—for example, how the staff interact through regular meetings, research presentations, and joint laboratory meetings. Therefore, how these teams add synergistic value to the division was not made evident.

Comments made to the panel by every group leader and by younger staff and postdoctoral researchers interviewed suggest that staff perceive the reorganization of the division to be a general success. Communication among the division management was reported to have improved. The groups are smaller than before, with an average staff of 8 to 10 people, allowing group leaders to devote more time to research and mentoring. However, there was insufficient information to permit assessment of the effectiveness of communication among the groups.

Research Groups

Cell Systems Science Group

The Cell Systems Science Group has as its vision to assist in the evolution of biology to a quantitative science and as its goal to model data on complex biosystems. Its focuses include stem cells, nanoparticles toxicity, imaging signaling pathways, and data and informatics. To accomplish its goals, the group has three core areas: bioinformatics, cell quantitation, and predictive models of complex processes. The group, which consists of biologists, biochemists, and bioengineers, is almost completely funded by STRS. While this cushions the group from large shifts in funding, it does not encourage the group to seek peer-reviewed recognition of its work.

The group has developed several innovative technologies that have potential for making a real difference to cell biology, but it has not yet been able to successfully engage outside groups such as the ATCC (the Global Bioresource Center) to achieve this goal. There is need for coordination between the group and the technology licensing office at NIST. A major challenge is the need for the laboratories to grow, not only within the group but through partnerships with other laboratories throughout NIST.

While the databases (HIV Structural Database, BIOFUEL Database, Bio Imaging Database, and Thermodynamics of Enzyme-Catalyzed Reactions) created within the group are well received, there is a need to move bioinformatics to a more forward position, which will require additional staff members who understand the domain. The group has done commendable work with the U.S. Food and Drug Administration (FDA) and ASTM International in the development of guidance documents for cell imaging. The group's biggest challenge is the possibility that funding could erode over time. One way that this challenge can be addressed is by partnering with other government agencies, including the FDA and the National Institute of General Medical Sciences.

Applied Genetics Group

The main mission of the Applied Genetics Group is to provide reference material for human, animal, and plant identification through genetic testing. The group has had a very successful program in partnership with (and funded by) the National Institute of Justice (NIJ). This work constitutes approximately 60 percent of the group's funding and should be stable for a number of years to come, because the group has met or exceeded the NIJ's expectations over the years. This work is widely recognized by the forensics community; the group leader is frequently invited to present talks and has written the definitive textbook on the topic.

The Applied Genetics Group needs to build on the significant base that it has established in developing technology and standards for DNA forensics. A number of opportunities are being pursued, including being part of a proposed national institute of forensic science. If such a center is created, NIST has to play a major role; therefore, the highest level of NIST management should be engaged in pursuing this opportunity. Developing standards (reference materials and databases) for clinical genetic assays may be another good opportunity, but there are many challenges that need to be overcome. One of these is overcoming the technical gap with the state of the art in sequencing technology. Short tandem repeat (STR) may be state of the art for forensics, but is old technology for the rest of the genomic field. The sequencing technologies are evolving exponentially, and to maintain a state-of-the-art program NIST will have to devote significant resources to acquire staff and equipment. A second challenge is that of overcoming regulatory hurdles. Working with clinical samples requires a considerable amount of regulatory and legal approvals; at present, NIST appears to be hesitant about and very slow in granting these. Another challenge is to address the lack of clinical partnerships. The group identified two examples (Huntington's disease and cytomegalovirus) where work has started in these areas, but a considerably larger effort will be needed to identify the clinical applications for which NIST can provide unique value. Partnering with clinical researchers will be helpful in identifying relevant clinical problems. The group should form a strategic partnership with NIH to identify areas of unmet need and opportunities for future funding.

The Applied Genetics Group has suggested forming a partnership with the ATCC to help them improve quality control of cell lines; this is an excellent opportunity and would be a great fit for this group. A successful NIST program in this area would result in saving significant amounts of money and time for experimenters relying on these cell lines for their work.

Macromolecular Structure and Function Group

The Macromolecular Structure and Function Group (MSFG) has as its charge to develop novel measurement methods and models to assess structure and function. The work in this group has applications in drug discovery, homeland security, protein engineering, biomanufacturing, and nanotechnology. The group is housed at the Center for Advanced Research in Biotechnology (CARB) and consists of seven staff scientists and one NRC Fellow. (CARB is a partnership among the University of Maryland Biotechnology Institute, NIST, and Montgomery County, Maryland.) The efforts of the group are augmented by one PhD student and five postdocs in the laboratory at the University of Maryland. While the MSFG receives impressive core funding from STRS, it also is able to apply for NIH grants through CARB and thereby to increase its total available dollars for research. The group was awarded $5 million in stimulus funding through the American Recovery and Reinvestment Act of 2009 (Public Law 111-5) to purchase an ultrahigh-field 950 MHz NMR system and has access to standard as well as state-of-the-art protein analytical instrumentation. The investment made in this quality of equipment will require a dedicated staff person to ensure that it retains its value. Given the real need in the biological and medical communities for solid standards for follow-on biological drugs, this is an important investment for NIST.

The MSFG is involved in a variety of research projects, including the processing of signal proteins and complex assemblies, ribonucleic acid (RNA) binding proteins, biological membranes and membrane proteins, and glycoproteins and biologics. Group members have also begun to investigate "green" (environmentally friendly) protocols for processing carbon nanotubes and are in the process of patenting and licensing the technology. Despite its many successes, the group has significant challenges. It must make strategic hires to remain competitive. More funding is needed to develop the biologics program fully. Because CARB provides off-site facilities, there needs to be more effort in harmonizing and maximizing the multi-institutional relationships involved.

Multiplexed Biomolecular Science Group

The vision of the Multiplexed Biomolecular Science Group is to use its expertise in physical and chemical sciences to enable genome-scale multiplexed measurements of biological systems. The group proposes to do so by developing infrastructure for standards and measurement science tools. The major efforts in the group are in the application of metrology to microarray data analysis and in microfluidics. Emerging programs include next-generation sequencing, the development of microbiological genomic standards, and metrology for multiplexed disease signatures.

This group is the most innovative in the division, as evidenced by the large number of publications, two Innovations in Measurement Science (IMS) projects (the only two in the division), and most of the patents in the CSTL. The IMS on microarray metrology is ending this year and was an extremely successful program. It led to the formation of the External RNA Control Consortium, hosted by NIST and its participants, which includes virtually every major genetic-analysis instrument and reagent manufacturer, many pharmaceutical and diagnostic companies, and numerous federal agencies and universities. This effort also resulted in the inclusion of sequence as a certified property by the International Organization for Standardization (ISO).

Another major effort of this group is the application of microfluidics technology to develop novel protein separation and quantification techniques. This team is innovation-driven and is charting its own course, somewhat independently of the mission of the division. While there is no doubt about the technical quality of this team's work, its alignment with the mission was unclear to the panel. Microfluidics is a strong capability for NIST, and the management and the researchers should find a better fit with the mission of the division.

While the current work of the Multiplexed Biomolecular Science Group is of very high quality, its plans for future work were not as concrete and clear. The group intends to become a major player in next-generation sequencing, metrology for disease signatures, and single-cell transcriptomics, but no concrete plans were presented to identify the unmet need or the driving biological or clinical problem, overall goals, and alignment with the NIST mission. The group does not have the critical mass of expertise in either genome biology or bioinformatics to match or exceed the state of the art in biomarker discovery, next-generation sequencing, or single-cell transcriptomics.

Bioassay Methods Group

The Bioassay Methods Group pursues research into new bioassay formats and materials, promoting standardization and defensible measurement claims through methods optimization and validation. This group also provides standard reference materials and reference data to support a broad range of health-, defense-, environmental-, and energy-research-related customers. This is the largest and most diverse group in the Biochemical Science Division, and as such it faces strong challenges in terms of the management of personnel and resources. The group has strong technical leadership, but the effort lacks a coherent vision statement.

The Bioassay Methods Group has a good mix of funding from core sources and external sources. Of all of the groups in the Biochemical Science Division, this one displays the best balance between the research and the traditional NIST mission of generating standard reference materials. The current mixture of employees, however, relies too heavily on contractors. Further, a long-term plan is needed to transfer the expertise and knowledge from the retired NIST cohort to the rest of the group.

The task of generating reference materials is nicely represented here. In order for the reference material and database area to flourish, the leadership of NIST must continually place adequate emphasis on these tasks and incentivize employees, including postdocs, for supporting this key function.

There are several areas of growth that this productive group could explore in order to increase its influence. A vision statement should be developed to encompass the major activities of the Bioassay Methods Group and allow for a continued balance between research and SRM activities. The criteria to evaluate employee performance may place greater emphasis on service, patents, publications, fundraising, and, more importantly, generation and support of SRMs. Alternatives to the Hirsch index (which measures the impact factor of publication) should be considered. The exact focus for the biofuel activities should be explored and optimized. Instead of defining standards for biofuels that may not have large economic impact, the group could partner with the leaders in the field and move its effort toward generic methods for biofuel standard classification. As another growth area, the Bioassay Methods Group should place more emphasis on protein measurements. Current efforts for protein characterization in other NIST divisions focus on structural aspects of protein characterization. The bioassay elements of protein measurements are not well covered by other NIST efforts, but they are key to homeland security and to clinical and general research activities.

DNA Science Group

The DNA Science Group has achieved highly significant results and recognition for its research in oxidatively induced DNA damage and repair. These research accomplishments reflect a long-term investment at NIST in a relatively specific area that integrates deep understanding of mass spectrometry and genetic science. Today, changes in DNA structure are more important than ever, as researchers can potentially develop new biomarkers, diagnostics, and therapies employing this understanding, and these advancements should continue through appropriate external partnerships. Within NIST, there is opportunity to extend these core competencies in mass spectrometry and DNA biochemistry across other project areas and applications that could benefit by this expertise. The group’s strong team and leadership could help enable this broader influence and impact. Retirements have led to key gaps in other parts of the division, and it is important that NIST leadership ensure that the group leader’s expertise propagates to his team.

Crosscutting Research Team

Nanotoxicity

Nanoparticles represent a globally important area in need of improved, more standardized measurement methodology. Toxicity, the focus identified within the Biochemical Science Division, is especially relevant as these new components are becoming increasingly prevalent in advancing materials, electronics, and life science and health care applications. The emerging crosscutting program in nanotoxicity is encouraging, but current efforts may not be sufficiently focused or distinct to elevate NIST into a leadership position in this area. The division should develop a comprehensive view of the needs and efforts underway in the United States, Europe, and Asia in order to identify the unmet needs that could best be advanced by the talent and capabilities at NIST. Once that view is attained, NIST should set clear objectives and leverage across university, government agency (FDA, EPA), and industrial stakeholders to achieve its goals. Efforts should perhaps include organizing workshops or consortia for this scientific community.

INFRASTRUCTURE

It is encouraging that stimulus funding is being used to address some large equipment needs of the division, but this may not be adequate to ensure that the investigators will be operating at a state-of-the-art level. It is not necessary for NIST to have the best and finest of each type of instrument, given the quality of expertise nationwide. However, NIST is often the only group to apply many of these instruments and techniques to the analysis of a given material or method, so it is essential that the investigators in the Biochemical Science Division have access to top-level instrumentation. If funding is not available within NIST, it is critical that the division be willing to strike strategic partnerships with other divisions and, whenever possible, avoid the duplication of equipment and expertise. The panel believes that this collaborative spirit would also improve buy-in from other divisions toward the mission of the BSD, because those divisions would be better informed and would be stakeholders.

As noted above, the Applied Genetics Group must overcome the technical gap with the state of the art in sequencing technology. The sequencing technologies are evolving exponentially, and NIST will have to devote significant resources to acquire staff and equipment to maintain a state-of-the-art program.

The Macromolecular Structure and Function Group has received funding to purchase an ultrahigh-field 950 MHz NMR system and has access to standard and state-of-the-art protein analytical instrumentation. The investment made in this high-quality equipment will require a dedicated staff person to ensure that it retains its value; this is an important investment for NIST.

OBJECTIVES AND IMPACT

The role of the Biochemical Science Division as the home of biology within NIST needs to be strengthened. NIST, like many institutions, has embraced the concept that biology-inspired technologies are important going into the 21st century, but it has not yet assigned the leadership role to the BSD in this. The BSD has formed strong alliances with appropriate standards organizations in the extramural community, including academia (the Microarray Gene Expression Data Society), industry (ASTM International's Committee F04 on Medical and Surgical Materials and Devices), data management and database organizations, and the ISO (nanotoxicity). It is partnering with other institutions such as the Institute for Systems Biology. The BSD should develop similar strategic relationships NIST-wide. One possibility would be to provide internal review of all biologically related research projects being considered by NIST for funding. Another possibility is to establish a seed grant program in which members of the division partner with scientists in other NIST laboratories.

Importantly, the division needs to forge a unifying strategic plan and promulgate a vision that clearly reinforces its importance to biological activities and that elucidates the fact that the division consists of more than a concatenation of groups doing work in biology. Many of the BSD's groups are looking for new opportunities, but the interactions were initiated and managed at the group-leader level. It is always good to develop bottom-up interactions whenever possible, as is the case with the partnership with the National Renewable Energy Laboratory, but without an overall strategy the likelihood of success is reduced. The BSD chief should work with her group and team leaders to establish a unifying strategic plan that reflects input at all levels.

CONCLUSIONS

Overall, the depth and breadth of the research program in the Biochemical Science Division are impressive. The division leadership and staff share a common vision. It is important now to articulate this vision upward throughout the NIST management group and to assert the central role of the division in biological standards and technology. This may require additional strategic hires, particularly biologists and clinicians to complement the bioengineers and analytical chemists. Partnering is another approach that should be considered. This can be achieved by developing consortia that include the medical community and industry. NIST is not structured to deal with human tissues and human clinical trials. Perhaps the division could best contribute by serving as a calibrator and developer of standard reference materials and methods.

The Biochemical Science Division should identify what it considers to be success in the context of NIST. There may be too many small efforts to make a major impact. An overarching strategy should be articulated and priorities set, based on identifying what kinds of activities can best be done in the NIST environment. Many of the groups have done this, but a top-down alignment of research with the division mission is missing. Once this is achieved, the management team will have less difficulty in sifting through the projects to determine which are the most important to pursue going forward.

Specific recommendations are as follows:

1. The nanoparticles research should focus on toxicology and should identify the most important problem for NIST to solve. Technologies for assessing the quality of nanoparticles are needed. The group should focus on what is happening in the broader community and should connect with it. This crosscutting team is close to being a core program within the division. The group needs strong input from

FDA/Environmental, Health and Safety, as well as input from clinicians and industry.

2. The Cell Systems Science (CSS) databases are good, but they need strengthening with respect to bioinformatics. The studies on fluorescence imaging address an important problem. The staff at that laboratory should be a focus on setting standards and quantitative methods for doing assays. Similarly, the microfluidics laboratory should consider the development of protocols and standards. Overall, the Cell Systems Science Group has strength in the quantitative measurement of cells, but there is need for more external validation of the group's work through extramural funding.
3. The Applied Genetics Group is well aligned with the NIST mission and is a model for group funding. If the overarching mission of the division includes medicine, this group should strengthen its applications to the medical community through the Centers for Disease Control and Prevention and to the ATCC.
4. The DNA Science Group's work in DNA damage and repair is among the best. The group should take the opportunity to collaborate with other groups, particularly with respect to biological mass spectrometry. A leadership transition plan is needed.
5. The research in the Macromolecular Structure and Function Group is outstanding. This group is a model of creative partnering, but it is important that the CARB laboratory fully embrace the NIST mission. NIST should clarify what it wants for its impressive investment in this laboratory. This group should address the issue of biosimilars (versions of existing biopharmaceuticals whose patents have expired).
6. The Bioassay Methods Group is the largest in number of staff, but it relies on contractors, perhaps too much. This group provides the best balance of science with measurement standards within the division. It may not be necessary to use senior scientists' time for this when technical staff can do the follow-through more effectively. The leadership should develop a forward-looking vision to unite the SRM teams with the research teams.
7. The Multiplexed Biomolecular Science Group has diversified funding and has successfully competed for two IMS grants. This group is making an impact on the field outside NIST with respect to microarrays. By interacting with other laboratories in the division, the group should broaden its expertise to include proteomics.
8. Overall, the microfluidics competence within the Biochemical Science Division is excellent, but it may not be being used to its greatest advantage. The management team should consider how to better align this expertise with the NIST mission.

4

Chemical and Biochemical Reference Data Division

SUMMARY

The Chemical and Biochemical Reference Data Division (CBRDD) performs experimental, theoretical, and computational research on the identity and reactivity of chemical species, emphasizing data, information, and protocols for the identification of chemical and biochemical species. The CBRDD provides critical databases for research and industrial process design.

Division programs fit well with national priorities and NIST focus areas. The CBRDD is a critical national and international resource. The division, in concert with the leadership of the Chemical Science and Technology Laboratory, has moved swiftly and thoughtfully to help meet urgent national and global challenges. The division's databases are essential for process design in existing, nascent, and future industries. These databases are used heavily by researchers throughout industry, government laboratories, and academic institutions. The NIST Chemistry WebBook (a Web site [http://webbook.nist.gov/] used by scientists, engineers, educators, and the general public, which provides access to a range of physical and chemical property data on chemical species and reactions) receives more than 2 million views per month. The division's research programs are addressing some of the most pressing problems of the present time: energy supply (biofuels) and utilization (combustion modeling); global climate change (atmospheric chemistry of global warming gases and aerosols, and possibly carbon cap-and-trade metrics); and health care (standards for diagnostic tests and for therapeutics).

The groups within the division are working well with one another and with other divisions on problems of mutual interest. This is particularly evident in the testing of experimental data against theoretical results. The overall mood of CBRDD staff appears to be strongly positive, with researchers who are dedicated to maintaining and enhancing the international stature of NIST. The creation by the CSTL of Division 832 (CBRDD) from the Gaithersburg, Maryland, portion of CSTL's Division 838 (Physical and Chemical Properties Division) appears to have been seamless. Researchers in Division 832 are pleased with the improved accessibility of management, and managers benefit from the reduction of travel between the Gaithersburg and the Boulder, Colorado, sites. The panel found numerous examples of continued and productive collaboration between the two sites. The work of the division is well focused and on target, and its quality, quantity, and impact are excellent.

TECHNICAL MERIT

The Chemical and Biochemical Reference Data Division is composed of 3 groups (Chemical Reference Data, Computational Chemistry, and Combustion and Kinetics), with 34 staff members (31 technical staff and 3 office support staff) and a number of postdoctoral associates and guest researchers. The division has 2 NIST Fellows and 1 Scientist Emeritus. The division's operating budget is approximately $9.95 million (40 percent appropriated, 49 percent measurement services, and 8 percent from other agencies). In 2007, division researchers produced 25 publications and gave 9 talks and 5 poster presentations. In 2008, division researchers produced 21 publications and gave 33 talks (2 invited) and 4 poster presentations; 15 publications are in press, have been submitted for publication, or were published in 2009.

Chemical Reference Data Group

The Chemical Reference Data Group is providing a unique and highly valued service to scientists and engineers in all types of institutions worldwide. The group continually strives for accuracy and validation of its standard reference data (SRD), as well as the completeness and user-friendliness of its services such as the WebBook and its participation in InChI (International Chemical Identifier, an International Union of Pure and Applied Chemistry [IUPAC]-supported, molecular identification methodology). The Mass Spectral Library remains highly regarded and in demand by the professional community (academe, industry, government). Outside revenues from the library constitute 48 percent of the division's total revenues from sales of standards. The proteomics project is forward looking, setting a goal of standardization of peptides and genetic markers similar to what has been achieved for simple molecules. The excellent collaboration with the theory group in constantly testing theory and experiment against each other and in the providing of data of established accuracy from both sources is a great strength of NIST's contribution to research and to industrial process design.

Computational Chemistry Group

The Computational Chemistry Group has evolved into a group that provides essential information to support the experimental programs in the Combustion and Kinetics Group as well as providing the fundamental data and theoretical support to the data analysis groups doing fluid simulation studies in Boulder. The group has many overarching responsibilities in the Chemical and Biochemical Reference Data Division. It has technical expertise in the areas of quantum chemistry method development and of statistical mechanics. These areas allow breadth of coverage of a range of chemical problems that span from atomic to macroscopic scales.

The group has made two significant advances: (1) it has developed a new Huckle-Density Functional Tight Binding method that has better parameterization and is more efficient for calculating molecular properties of large molecular systems, and (2) it has developed an efficient new method that can examine electron conductance in molecular systems. This advance has reduced computational times from months to minutes, and the software is platform-independent.

In two areas, new personnel would assist the group in addressing problems related to NIST's current mission. One area not fully covered by the group is expertise in dynamics of chemical processes. For example, a new hire in the area of quantum dynamics would provide an important bridge of expertise within the group as well as expand the kinds of problems that the Computational Chemistry Group can tackle within the division. Currently the group has expertise in density functional but not semi-empirical methods for the computation of fundamental properties of known accuracy for molecular systems larger than 50 atoms.

Combustion and Kinetics Group

The Combustion and Kinetics Group has maintained its historical excellence and has moved forward aggressively to meet the new challenges of the 21st century (e.g., programs on Real Fuels, Photochemistry of Global Warming Gases, and potentially the Chemistry of Atmospheric Aerosols). It is setting the standard for excellence and precision for shock-tube studies of combustion chemistry and for the reactions of hydroxyl (OH) radicals. The shock-tube studies of the decomposition of (present-day and alternative) fuel molecules and of the radicals so formed are critical for predicting the performance of fuels and engines for the future. The measurement of diffusion coefficients as well as reaction rate constants for both stable and reactive species is critical for the simultaneous treatment of chemical kinetics and turbulent flow in real engines. The production of a database for the pyrolitic decomposition of all linear hydrocarbons is a major contribution.

The atmospheric chemistry of global warming gases, especially their reactions with OH, must be modeled accurately in order to predict global climate. The careful measurements of rate constants for reactions over the full range of atmospheric temperature and pressure are another major contribution of this group.

The proposed work on aerosols for potential assessments of global warming should be pursued vigorously. The aerosols field is badly in need of measurement techniques and standards. Aerosols are a serious missing piece in models of atmospheric chemistry for both global warming and air pollution and are important in the performance of combustion engines.

The group's Gas Phase Kinetics Database is heavily used and will have great value for many applications in coming decades. Although it is very useful in its present form, it is a compendium (no evaluation) that would benefit from evaluation to prune out mistakes and from some work to add more data. An increase in effort level would have substantial value.

With respect to metrics, the CBRDD reported 20 journal articles published in calendar year 2008 by its staff, which includes 21 PhDs. There were 32 talks and presentations at meetings, only 2 of which were noted as invited. Members of the division were not among the award recipients reported by the CSTL.

For the division, and for the CSTL overall, there should be more emphasis on refereed publications and on invited talks. There also should be more effort made to encourage staff to pursue, and to help them attain, external awards. Many staff members should be fellows of the American Physical Society, the American Association for the Advancement of Science, the American Chemical Society, and numerous other professional organizations. Awards from such organizations are useful stepping stones to other national professional awards.

INFRASTRUCTURE

Access to the databases of the CBRDD is interrupted by network shutdowns, which happen unpredictably, for periods of time as long as 6 to 12 hours. These interruptions limit access to the database for reference by the outside community and by the staff for making necessary upgrades to the database. These databases are used internationally and must operate with 100 percent reliability "24/7"; anything less is a serious blemish on the credibility of the United States as a technology leader among nations.

The Chemical Reference Data Group is adequately staffed and supported. The laboratories appear to be in very good repair and well maintained. Equipment for the group is leading edge (e.g., Ion Trap/Quadrupole Time of Flight) and in good working order. There are, however, significant opportunities for important improvements in some of the databases, a number of which are supported by a 0.5 FTE or less effort. The overall effort level on the databases in the division might be improved by more positive recognition for these activities by NIST management.

The Computational Chemistry Group could use two new staff members to help it address problems related to the dynamics of chemical systems and to provide accurate fundamental property information for large chemical systems. These two hires would help the group meet its overarching responsibility for providing accurate data for groups within the division.

The instrumentation and personnel for conducting shock-tube experiments have almost entirely fallen out of use in the United States. This experimental tool, in the hands of the Combustion and Kinetics Group, is the way to obtain quantitative chemical information at combustion temperatures and pressures. Historically, shock tubes have been a laborious and imprecise way to obtain reaction rate constants and mechanisms. Therefore, it is critical to provide the best possible equipment for tackling 21st century combustion and atmospheric chemistry problems. The new shock tube designed for studying soot and polyaromatic hydrocarbon (PAH) formation in combustion should be of the highest priority.

Equipment is needed for new experiments in order to provide measurement standards for aerosols and data on aerosol chemistry, particularly as it relates to climate change. This is a high priority for NIST's mission.

The 1960s buildings of the CSTL are badly in need of renovation, which should be funded promptly. If this is not done, a great deal of time and money will be wasted in attempting to operate safely and productively with dysfunctional building systems. Scientists should be an integral part of the design effort so that research can be carried out safely and efficiently in compliance with modern standards.

OBJECTIVES AND IMPACT

The expressed goals of the Chemical and Biochemical Reference Data Division include the following:

- Provide databases on the properties, thermodynamics, reactivity, and rate constants for chemical species, from atoms and small molecules to biological molecules and nanoparticles;
- Distribute electronic databases and software in a manner that is convenient to NIST's customers;
- Establish validated databases for peptides and proteins to enhance proteomics research and development;
- Use theory and experiment to improve the understanding of the underlying physics and chemistry of peptide ion fragmentation in order to provide more robust procedures for inferring the identity of a peptide ion from the masses and abundances of its fragments;

- Work with the IUPAC to perfect the InChI data standard;
- Provide quantitative and accurate data from theory and new experiments that complement and test existing experimental data;
- Provide theoretical support for NIST work in data evaluation and chemical property measurements;
- Provide state-of-the-art theoretical tools that are tested against the best experimental data to establish their accuracy and reliability;
- Develop resources to provide guidance to non-experts on theoretical methods;
- Provide databases and tools for chemical reaction rates and transport processes for atmospheric and combustion chemistry modeling to support the design of new combustion engines, efficient combustion equipment, and effective climate change reduction strategies, and the study of atmospheric pollution. Support applications to alternative fuels and global warming; and
- Provide a consistent, high-quality compilation of solvation thermodynamics data for a set of pure fluids.

The potential impact of success in the CBRDD's research areas is critically important to the nation with respect to the areas of energy, climate change, and health. There are several examples in the division of research programs that could have a very large impact.

The Computational Chemistry Database is an important resource for researchers. It has become an essential database of computational chemical information for many chemical species for which experimental data are lacking. One of the challenges to people in universities and industry who want to use the Computational Chemistry Database is that of obtaining access to it. The Computational Chemistry Database should be integrated with the WebBook database. Currently they are only loosely integrated; together on the same platform, however, they would provide users with a more powerful tool. As a temporary measure, both the WebBook database and Computational Chemistry Database could be displayed on the same Web page as a resource of chemical property information for users from universities and industry. It may be beneficial to merge the Process Informatics Mode (PrIMe) database at the University of California, Berkeley, into the WebBook as well.

Work on the identification and characterization of peptides and proteins could have a significant impact on the research on proteomics and its ultimate usefulness in health care.

Theoretical work on the decomposition of explosives in the solid phase is particularly impressive, since 30 years of extensive experimental efforts have failed to provide an understanding of this chemistry. The results are valuable, not only in the public safety and security program, but also more broadly for all military and civilian uses of explosives and energetic materials.

The collection of shock-tube rate-constant data to build a rate-constant database for the pyrolytic decomposition of all linear hydrocarbons is an exceptional accomplishment for its basic scientific elegance and its practical value in designing combustion systems and evaluating the environmental impact of alternative fuels.

The temperature-dependent OH reaction-rate data for global warming gases are an essential component of predictive models of climate change.

CONCLUSIONS

The panel presents the following conclusions and recommendations with respect to the work of the Chemical and Biochemical Reference Data Division.

The leadership of the division (that of the division chief and the group leaders) is very good; it demands high-quality work and continuous productivity, supports its staff, and maintains a positive outlook. The work of the division is well focused and on target; its quality, quantity, and impact are excellent. Though there are some gaps (for example, the overall database effort and the Computational Chemistry Group), the professional staffing is very good; the scholarship and dissemination (publication and databases) of internal work is high-level; with two NIST Fellows, the division's excellence is recognized. Additional personnel should be considered for the Computational Chemistry Group and the Chemical Reference Data Group.

Renovations of the buildings occupied by the division should be completed promptly. Important equipment for shock-tube and aerosol work should be provided. An information technology policy change at the NIST level is required in order to prevent interruptions to the servers that support the databases and WebBook.

The Computational Chemistry Database should be integrated with the WebBook database.

With the substantial number of new projects, the new administration's priorities, and the improved budget, a more comprehensive strategic planning exercise is warranted, preferably together with all of the CSTL and NIST.

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Process Measurements Division

SUMMARY

The Process Measurements Division's (PMD's) mission of disseminating national measurement standards for thermodynamic parameters and conducting relevant measurement science research fits well with national priorities and NIST focus areas. The PMD provides essential calibration services in fundamental parameters that support many sectors of the U.S. economy as well as facilitating international commerce. It conducts research that is directly aligned with NIST and national priorities. The PMD's research includes projects that support the Department of Homeland Security (microsensor chemical detectors), the climate-change research community (spectroscopy and gas properties), the biopharmaceutical industry (gold nanoparticle reference materials), and developers of the hydrogen economy (hydrogen gas data and flow-rate calibrations and standards). In those areas for which the PMD maintains U.S. national standards and provides measurement services, it is preeminent among national metrology institutes; the division is an important national resource. The overall mood of the PMD staff appears to be positive, with researchers dedicated to maintaining and enhancing the international stature of the division.

RESPONSE TO RECOMMENDATIONS FROM THE PREVIOUS REPORT

The panel's 2007 report[1] contained nine specific recommendations for the Chemical Science and Technology Laboratory. Those recommendations are reprinted below; each is followed by the panel's current assessment of the PMD's response to the recommendation.

1. The set of criteria known as 5+1 for ensuring that the research projects are aligned with the mission of NIST and the laboratory should continue to be used. The CSTL leadership should link its more basic research investments to the potentially important measurement-related outcomes that are envisioned to result from CSTL research.

   The PMD recognizes the need to spend more effort on this issue. The plasma processing project is a key example.

2. The CSTL leadership should put more effort into communicating to the staff the rationale for resource allocation between new initiatives and established programs, some of which produce revenues through standard reference materials (SRMs). One example is the current focus on nanoscience and nanotechnology, which competes with established metrology.

[1] National Research Council, *An Assessment of the National Institute of Standards and Technology Chemical Science and Technology Laboratory: Fiscal Year 2007.* Washington, D.C.: The National Academies Press, 2007, pp. 1-2.

The PMD has effectively transitioned several of its programs to the bioengineering arena.

3. CSTL should continue its practice of cross-pollinating research planning teams with individuals from different divisions as new initiatives are developed.

   The PMD has been participating in cross-divisional planning related to the focus in the biosciences area, and this participation has increased somewhat. Recently, the chief of the PMD has been tapped to coordinate the activity that NIST is planning and implementing in the area of carbon mitigation. This cross-divisional activity involves the Process Measurements Division and the Analytical Chemistry Division within the CSTL and several other divisions within NIST and other laboratories.

4. There is a sense that a greater fraction of research is being directed at computation than at experimentation and instrument development. The CSTL leadership should examine this trend to assess its impact on future capabilities of the laboratory.

   The PMD seems to have a good balance between modeling and experimentation. It has automated one of its measurement laboratories (Thermometry Laboratory) with impressive success. This is a good example of using modern computer techniques to save labor and improve efficiency, and it should be examined for other measurement laboratories.

5. CSTL should consider special efforts, such as interdivisional seminars and study groups, to generate more interest in interdisciplinary projects and to avoid redundancy in research projects across divisions.

   This remains an area for improvement within the PMD. It is a challenge, common to many technical organizations, to motivate researchers to participate in technical activities that are not closely tied to their personal areas of expertise and activity, but PMD management should continue to try to find ways to expand the technical interactions of its researchers.

6. The CSTL leadership should carry out its planned efforts to communicate to the staff the incentives for disclosing intellectual property and applying for patents.

   The PMD seems to be doing a good job in this area.

7. The ratio of Ph.D. scientists to technical and office support staff appears to be so high that the Ph.D. scientists are often required to perform a technician's work to accomplish a task. Besides serving as a barrier to the recruitment of outstanding scientists, this imbalance reduces the research productivity of the scientists. CSTL leadership should assess the ratio of support staff to Ph.D. scientists in terms of its effect on recruitment and productivity.

This ratio of support staff to PhD scientists is an obvious problem in the PMD. NIST is a very high-level intellectual organization, and therefore it is a common practice within NIST to strive for intellectual flexibility by focusing its hiring efforts on PhDs. It is also difficult to gain funding for established standards activities. However, considerable efficiencies could be realized with more support personnel, and improved basic research would be realized.

8. It is not clear that the laboratory [the CSTL] has developed guidelines for replacing scientists in critical areas who retire or leave the laboratory for other reasons. The laboratory should develop a strategic plan to address recruitment issues and identify areas of opportunity and areas of concern.

   The PMD seems to be doing a good job in this area.

9. The CSTL should increase efforts to make its scientists more visible in their respective scientific communities.

   Many of the top PMD scientists seem to have good external recognition; however, the PMD recognizes this as an area to be improved.

TECHNICAL MERIT

The Process Measurements Division is composed of five groups: Fluid Metrology, Process Sensing, Thermometry, Pressure and Vacuum, and Nanoscale and Optical Metrology. The division seeks to improve the realization of U.S. national measurement standards for temperature, fluid flow, liquid volume and density, pressure and vacuum, humidity, and airspeed. The PMD also seeks to develop the science to support new or improved measurements and standards technologies, with an emphasis on industrial process applications. The division provides access to these standards by providing instrument calibration services, SRMs, and standard reference data.

Overall, PMD staff are of very high quality, very sophisticated in their methods, and positive in their attitude about NIST and their work.

In the division’s measurements groups, most activities are among the best in their field, and they produce the secondary calibration tools and standards that are recognized as the best. These secondary standards are used by other nations for primary calibrations. The measurement groups have responded well to market needs, and their facilities allow the attainment of the highest standards of calibration to take place.

The pressure measurements team produces methods and standard calibration services for pressures down to 10^{-7} pascals (Pa). Methods for pressures as low as 10^{-11} Pa should be provided, because the semiconductor and solar energy processes frequently work in those pressure realms.

An example of work that the PMD has done very well is the pressure transfer standard. The PMD developed a transfer standard package (TSP) with high stability to be used as a way of comparing the performance of primary pressure standards from NMIs around the world. Typically, the TSPs use pairs of resonance silicon gauges, which are based on microelectromechanical systems technology; a temperature-controlled enclosure (based on a commercially available cooler with an incorporated thermoelectric cooling unit); support electronics; and customized software. The PMD developed a modification of the TSP as a prototype to provide NIST pressure traceability for the Army Primary Standards Laboratory (APSL) for pressures of up to 130 kilopascals (kPa). For its needs, the APSL requires a reliable barometric-pressure range instrument that is stable to within 50 ppm over a period of 1 year. This is to support calibrations for a wide range of precision pressure equipment—the most stringent requirement is the calibration of aircraft instrumentation calibrators. The PMD reports that, based on its experience with distributing TSPs internationally, the long-term calibration stability of this prototype will meet or exceed the Army requirement. The PMD expects these transfer standards, with their demonstrated stability, to remain within Army requirements for several years before they would be returned to the PMD for recalibration. This work is highly innovative, and the stability and precision of the standards are impressive.

The Thermometry Laboratory has undergone major renovations and is very impressive. The laboratory has been automated using LabView® software. The automation project was a pilot to see whether or not this approach would be useful, and it turned out to be a greater success than the PMD had expected. With the new system, several calibrations can now be carried out at the same time using far less technical staff time. Since tasks associated with calibration activities lend themselves well to automation, the PMD is concentrating on automation in this context at the moment. This example demonstrates that the automation of tasks that are repetitive and must be done in a particular way increases the efficiency of the laboratory and its staff. Other measurement laboratories should consider implementing this automation, using the same software and hardware platforms.

The sapphire high-temperature measurements pursued by the PMD are much needed by industry; the tool geometry specifications have been established by working with the end users. This is an example of a program that is well aligned with the NIST mission and should be completed. The program could have more impact and should be reviewed internally to ensure that it is staffed at a level sufficient to achieve its potential for impact.

The plasma processing effort is a technically solid program; however, the customer base has evaporated. This program should be refocused and better aligned with the NIST mission. There does not seem to be an established methodology to evaluate and eliminate programs within the PMD. It is recommended that the PMD management team establish such an evaluation program. This would make the program direction choices easier to implement.

Industry focus has been shifted away from semiconductors (a heavy emphasis in the past) into light-emitting diodes, the Smart Grid, and carbon cap-and-trade (energy-related) programs and the associated technologies.

The work involving quasi-spherical resonators to provide an atomic standard of pressure is impressive. The goal of the research involved here is to develop an accurate primary standard for pressure in the range of 0.3 megapascals (MPa) to 7 MPa, which is based on fundamental physical properties of helium and the use of quasi-spherical resonators. Using quantum mechanical theory, it is possible to predict the polarizability of helium, with agreement among all predictions of a few parts in 10^7. Quasi-spherical resonators have been developed that use acoustic and microwave resonances to measure the dielectric constant of helium from measurements of the microwave resonance frequencies of the cavity. Helium was used initially, but impurities in the helium presented a problem. Argon was then used, followed by the use of a mix of helium and argon. The approach of using quasi-spherical resonators has revolutionized the realization of pressure standards. Moreover, NIST and other

NMIs are using these cavities to determine imperfections in the internationally accepted temperature scale—the International Temperature Scale of 1990, or ITS-90.

The PMD is pursuing measurements for biopharmaceutical manufacturing, the objective of which is to develop standards and measurement tools to enable better comparability and more efficient science-based manufacturing of biological products. The manufacturing of protein drugs is expensive and inefficient; inadequate metrology results in high costs for these drugs. The researchers are using the technique of electrospray-differential mobility analysis to measure protein aggregation. The electrospray process, used in the past for separating gold nanoparticles of very precise dimensions, is now being used successfully in this new context. The team is using a technique that was employed for one type of particle, and bringing it into a biological application is commendable. This is a good example of transforming a program with less than good support into a program in a new arena (the biological arena) that is of interest today, and an arena in which it is good for NIST to be involved—one in which standards are anticipated to be increasingly important.

Protein aggregation can decrease the safety and efficacy of protein therapeutics (a category of biotechnological drugs), and the adsorption of protein therapeutics to bioprocessing materials used in the production, storage, and delivery may also contribute to this problem. A technique for surface analysis, x-ray photoelectron spectroscopy (XPS), is being used to attain elemental information on all of the elements on a sample (except hydrogen and helium). The objective of this work is to provide protein adsorption data, measured on materials commonly used in bioprocessing, to address these issues. Using this technique and the fact that there are surface interactions with proteins mean that the researchers have to understand how the particle changes with time. This is more complex than a mere physical measurement; the standard has to be understood.

The biological work of the PMD is impressive, and it is good for NIST to be doing work in the biological arena.

If a process is changed in biological and semiconductor processes, the process needs to be recertified. In the semiconductor manufacturing arena, the copy exact processes are well understood, and they assist in the scaling-up processes and the transferring of complete fabrication rules to new facilities. The ability to do this is based on well-understood metrology methods and standards, many of which are directly traced to early work at NIST. The division should explore ways to increase work directly related to methods and standards that are directly applicable to drug manufacturing in order to enable the cost-effective scale-up of processes.

In performing the chemical sensor work being pursued in the PMD, the researchers are very clever about how they extract data and carry out sophisticated analysis. The technology involved emphasizes the integrated, multidisciplinary approach, which has become more of a trend in this group. In order to realize the impact of technologies such as chemical sensors, there is a demand on many disciplines that must be carefully integrated to ensure success. It is encouraging to see the multidisciplinary approach—using a variety of technologies to deposit the sensory materials, using outside sources effectively, employing the properties of these materials by using rapid thermal cycling to achieve chemical fingerprints in a novel way, and taking the data and using computer modeling and analysis to extract data in a unique way. In addition, the background materials chosen are appropriate. This is an exciting technology, and the division should actively pursue external partners. It is encouraging that a research license already exists with an external company.

The work using calibrated nozzles for fluid-flow metrology is very good. It is elegant in its simplicity and precision, and this is a technology that is clearly appreciated by the international community. Other countries come to this group to have their standards certified as well.

In 2007, division researchers produced 68 publications, gave 56 talks, and had 7 patents pending, with 29 division staff members holding professional committee assignments and 2 holding editorships of professional journals. In 2008, division researchers produced 83 publications, gave 48 talks, and had the same 7 patents pending, with 28 division staff members holding professional committee assignments and 2 holding editorships of professional journals.

The Department of Commerce Silver Medal Award is the second-highest honor awarded by the department. It is bestowed for exceptional performance characterized by noteworthy or superlative contributions that have a direct and lasting impact within the department. One was awarded to division personnel both in 2007 and in 2008.

INFRASTRUCTURE

Of the Process Measurements Division laboratories visited by the panel, differences between the old and new buildings are apparent; however, even in the old buildings, no staff members complained about their space, so space does not appear to be a problem. There is a fair amount of aging equipment (old power supplies, for example), however. A review of capital equipment should be undertaken with an eye to ensuring that the most efficient and safest equipment is provided. NIST hosts numerous visitors from many countries, and the appearance of being state of the art is important.

As noted above, the automation of the Thermometry Laboratory is an impressive achievement. This involved the use of LabView® to fully automate calibrations, which, prior to automation, were tedious, time-consuming, and required considerable manpower. The automation of this laboratory should be a model for automating other measurements laboratories that have similarly routine (although important) measurement requirements. Moreover, there should be cross-pollination between the groups to avoid unnecessary duplication of efforts in laboratory automation. Considering that the PMD is looking at automating laboratories, the need for computer and automated equipment would be a good investment of resources.

The Pressure Laboratory is a state-of-the-art facility. There is a measured, large improvement in the accuracy of pressure measurements with the new facility.

With the recent rise in interest within the federal government in hydrogen as a potential part of the future U.S. energy landscape, NIST is anticipating that it may be expanding its role in hydrogen-related standards development. The PMD is designing a new facility for hydrogen-related activities. The safe handling of high-pressure hydrogen gas is, of course, a key consideration as plans for the facility move forward. Accordingly, the PMD is taking a careful, step-by-step approach in designing and planning for the new facility. Although it is not currently a certainty that hydrogen will become a more significant part of the future infrastructure of the United States or that hydrogen-related activities at NIST will increase significantly, the PMD is planning the new facility with an eye to the possibility that hydrogen may eventually be used there.

The current approach to safety is to initially qualify the new facility's operation for pressures of up to 6,000 pounds per square inch (psi), while also considering the requirements associated with the handling of high-pressure hydrogen. Initial activities will involve the use of argon or nitrogen, followed by the use of methane. Government efforts to use hydrogen as a fuel for vehicles may lead to the facility's being used to study the effects of transient flows on the response of typical flow meters, and the development of standards that account for transients. Currently, standards of this type are not available, although many realistic, real-world gas flows involve large transients. The PMD is planning to put as much of any combustible material as possible outside the building. This is a sound element in an approach to safety planning for this facility.

There is a critical need for full-time technicians, especially in those areas where measurements and calibrations are intense. In an effort to strive for intellectual flexibility, hiring at the PMD typically favors PhDs rather than technicians. Moreover, the way in which new funding comes into the PMD does not generally support the established standards activities, and the division does not have a method for keeping those activities' funding at a healthy level as compared with funding for high-profile research areas. The PMD, in concert with its NIST leadership, needs to specify the ways in which NIST evaluates and values the long-standing standards activities of the PMD. There does not appear to be a strategy for maintaining the ranks of technicians at a healthy level. The addition of a few technicians would probably greatly improve the productivity of the most senior professional staff—taking advantage of the investment that the PMD has made in them. Therefore, there should be more technicians to improve the efficiency of the entire technical staff. There are many examples of PhD-level personnel doing routine functions, and the addition of more technicians would free the PhD-level staff to perform more PhD-level work.

OBJECTIVES AND IMPACT

The PMD should consider and investigate media opportunities to publicize the usefulness of its capabilities. Many more potential users of PMD services and products would come forward if they knew more about what the PMD has to offer. In addition, industry would probably take more advantage of PMD capabilities if the cycle time for standards work were shorter. Also, the division is slow when it comes to developing a new process for a standard, which inhibits industry with respect to using PMD services. Finally, the PMD should continue to check for and evaluate new technologies that may be coming in the future and should plan for how its capabilities would properly address them.

CONCLUSIONS

Overall, PMD staff are of very high quality and very sophisticated in their methods, and they evince a positive attitude about NIST and their work. Among the PMD's measurements groups, most activities are among the best in their field, and these groups produce the secondary calibration tools and standards that are recognized as the best.

The automation of the Thermometry Laboratory, using LabView® software, is an impressive accomplishment. Other measurement laboratories should consider implementing this automation, using the same software and hardware platforms, and there should be cross-pollination between the groups in order to avoid unnecessary duplication of efforts. Since the

PMD is looking at automating laboratories, computer and automated equipment would be a good investment of resources.

Methods for pressures as low as 10^{-11} Pa should be provided by the PMD, because the semiconductor and solar energy processes frequently work in those pressure realms.

PMD management should establish an evaluation methodology and program to facilitate the elimination of programs when they are no longer effective in meeting the PMD and NIST missions. The plasma processing effort is an example of PMD management's recognition of this need.

The sapphire high-temperature measurements pursued by the PMD are much needed by industry. The program could have more impact and should be reviewed internally to ensure that it is staffed at a level sufficient to achieve its potential for impact.

The PMD has transitioned several programs to the bioengineering arena very well. It is good for NIST to be doing work in the biological arena, where standards are anticipated to be increasingly important. The PMD should explore ways to increase work directly related to methods and standards that are directly applicable to drug manufacturing in order to enable the cost-effective scale-up of processes.

The PMD should consider and investigate media opportunities to publicize the usefulness of its capabilities. Many more potential users of PMD services and products would probably come forward if they knew more about what the division has to offer. Industry would probably take more advantage of PMD capabilities if the cycle time for standards work were shorter. Also, the PMD is slow when it comes to developing a new process for a standard, which inhibits industry with respect to using PMD services. The PMD should continue to evaluate new technologies that may be coming and plan for how its capabilities would address them.

Although many of the PMD's top scientists seem to have good external recognition, the division should continue its efforts to make its scientists more visible in their scientific communities. It is a challenge to motivate researchers to participate in technical activities that are not closely tied to their personal areas of expertise and activity, but PMD management should continue to try to find ways to expand the technical interactions of its researchers.

With increased interest within the federal government in hydrogen as a potential part of the future U.S. energy landscape, NIST is anticipating an expanded role in related standards development. Although these possibilities are not a certainty, the PMD is planning ahead for a facility to accommodate the safe handling of high-pressure gases, with an eye to the possibility of eventual hydrogen use. The panel thinks that the careful, step-by-step approach being taken by the PMD in designing and planning for the new facility is sound.

There is a critical need for full-time technicians, especially in those areas where measurements and calibrations are intense. The addition of a few technicians would greatly improve the productivity and efficiency of the entire technical staff.

A review of capital equipment should be undertaken with an eye to ensuring that the most efficient and safest equipment is provided.

6

Surface and Microanalysis Science Division

SUMMARY

The mission of the Surface and Microanalysis Science Division (SMSD) is to serve the nation in areas of chemical metrology, research, standards, and the acquisition and analysis of data. The SMSD provides excellent service to the U.S. government and the United Nations through the identification of radioactive and explosive materials as well as the setting of sample standards and development of analytical methods. SMSD research includes a wide range of topics that are critical to the maintenance of national standards and measurement science for the nation. The division is well supported with respect to equipment, facilities, and budget. Supported by both core NIST funding and other agency funding, the division maintains an appropriate balance between the goals of making progress on longer-term problems not amenable to quick solutions and producing results in current areas of interests that enhance the profile of NIST. The morale of the SMSD staff is positive. The researchers are dedicated to the goals mentioned above. This division is an important national resource.

RESPONSE TO RECOMMENDATIONS FROM THE PREVIOUS REPORT

In the panel's 2007 report,[1] a few minor suggestions were given for further improving the existing high-quality projects of the SMSD. These included better theoretical support for projects involved in the detection of explosive materials, better definition and evaluation of the health and safety risks of nanoparticles, improved theoretical understanding of cluster secondary ion mass spectrometry (SIMS) of organic layers, more extensive collaborations in the clean-room facility with experts on the synthesis and theory regarding the fabrication of molecular electronics, and maintenance of the highly valuable data concerning surface electron microscopy.

The majority of the suggestions have been accepted and implemented by the division. For example, a detailed study that involves the preparation and quantitative analysis of standard explosive samples was done. The fundamental properties of explosive molecules have also become better understood since the 2007 review. The transport of nanoparticles in biocells has been delineated. Sputter SIMS analysis of biomaterials was carried out. A semitheoretical study of the organic thin-film transistors fabricated by a device group in another NIST division has been completed. The highly popular x-ray-analysis database that was based on the Apple computer system has been updated to a personal computer system. Additional work on theory, modeling, and simulation should be done, perhaps in collaboration with experts in other divisions of NIST.

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[1] National Research Council, *An Assessment of the National Institute of Standards and Technology Chemical Science and Technology Laboratory: Fiscal Year 2007.* Washington, D.C.: The National Academies Press, 2007.

TECHNICAL MERIT

The two major objectives of the Surface and Microanalysis Science Division are the development of metrology technology and fundamental scientific research. For the former, five representative topics were demonstrated to the panel. These are as follows: the identification of uranium (U) isotopes, the detection of trace amounts of explosive materials, chemical mapping by desorption mass spectrometry, the tracking and removal of nanoparticles in aquatic environments, and the correlation of cracks in concrete with chemical mapping by high-resolution transmission electron microscopy (TEM). For the latter, three representative topics were shown: chemical imaging of individual nanostructures, mechanisms of charge transfer in molecular nanoelectronics, and super-resolution leading to significantly improved optical microscopy. The division's scientific program appears to be larger than that for technology development simply because the scientific projects have more subtopics. However, the technical studies are well targeted at solving problems in national and international security, environmental protection and sustainability, and transportation infrastructure. All of these are national priorities with high impact and high visibility.

The scientific studies are spread over a wide range of fields in chemistry, bioscience, optics, electronics, materials, and nanotechnology. The accurate identification of trace isotopes of U is unique and critical to DHS and International Atomic Energy Agency (IAEA) missions. The development of trace-detection metrology for explosives is important to national security. For this purpose, a detailed method for the preparation of standard samples has been investigated. The need now is to establish expected sample lifetimes. The integration of chemical analysis techniques would also be beneficial.

The work on high-throughput, site-specific chemical mapping by SIMS is of practical value to airport security. The reliability of the process and the long-term effects on health may need investigation.

The quantitative chemical imaging of individual nanostructures by TEM is interesting and potentially important for applications to both safety and the environment. It may also have benefit for potential applications to microelectronic devices—for example, in helping to understand Si/high-k-dielectric interfaces. The focus on the development of robust methods of analysis and energy-dispersive techniques for aberration-corrected TEM (in contrast to efforts in electron-energy-loss spectroscopy in other national laboratories) is consistent with the NIST mission of metrology development.

The project on studying engineered nanoparticles in aquatic environments is potentially important for water purification. An effective agent, such as a chelator, may help in separating carbon nanotubes from the aquatic environment.

The cadmium selenide (CdSe) quantum-dot project, measuring the trophic transfer of nanoparticles in a simplified invertebrate food web, indicates that the biomagnification of nanoparticles, or at least particular types of nanoparticles, may not represent a health hazard. A further study on why the nanoparticles do not accumulate will enhance the visibility of this project.

The fast TEM imaging on the formation of cracks in concrete is very good work with practical value. A detailed analysis of the connection between the chemical distribution and crack formation would be an excellent scientific study. More generally, by addressing the analysis of large specimens and connecting micro and macro properties of complex materials, this work can have a broad impact on detailed characterization and its relationship to the performance properties of a wide variety of complex materials.

The work on charge-transfer mechanisms and the probing of surface potentials in nanoelectronics is interesting. The emphasis on developing reliable methods and databases for molecular electronics is appropriate in view of the NIST mission.

When completed, the project involving super-resolution optical microscopy will have particularly high impact. The principal investigator has already published several excellent papers on this subject.

The overall technical quality of the division is very good, with many projects being among the best. However, the impact of SMSD's work could be enhanced significantly without the need for major additional resources by adding theoretical support to some of the experimental projects. This could be accomplished, for example, by initiating collaborations with outside organizations. It is encouraging that many of the research projects already involve other divisions in NIST; external government agencies such as the U.S. Air Force, Department of Homeland Security, National Institutes of Health, National Cancer Institute, Food and Drug Administration, Savannah River National Laboratory, and various Army laboratories; industry, including General Electric and SEMATECH; and universities such as the University of Maryland, Pennsylvania State University, and the University of Kentucky. Given the present imbalance between the number of technical staff and the relatively large amount of state-of-the-art equipment, the impact of the division could be made even more impressive by establishing more collaboration with outside organizations such as universities or national laboratories. It can also be anticipated that such collaborations would bring in fresh ideas, and the existing excellent infrastructure would be used to explore new territory.

A division-wide strategy needs to be developed to enhance the visibility of the SMSD and its impact in the government and scientific communities, because this division includes a wide range of activities. Some projects can benefit from an improved definition of strategy, such as the long-term direction of scientific study and technology development. The division should also promote worthy investigators for external recognition in the form of prizes and awards.

The scientific staff of the division is highly productive. For example, in fiscal year (FY) 2008, division researchers produced 55 manuscripts for publication, made 118 presentations that included 53 invited talks, filed for 1 patent, received 3 awards including 1 fellowship, and participated on 110 committees, including serving as committee leaders. Every member of the scientific staff is involved in the publication and presentation process, with a few members compiling outstanding records. On average, each member of the scientific staff published 1.7 papers and delivered 3.5 talks. This is an excellent record, which shows that the division is meeting its mandate to make a difference in scientific and technical areas.

INFRASTRUCTURE AND SUPPORT

Compared with most university and industrial research laboratories, the Surface and Microanalysis Science Division has some outstanding experimental equipment. Most of it can be considered top of the line. Laboratory space, utilities, and safety features are all significantly better than what is found in many other laboratories. Although the equipment may not be used to full capacity, as noted above, the scientific and supporting staff engaged in the research and service programs are outstanding. The use of additional graduate and undergraduate students in the summer is also a positive strategy whose continuation is encouraged. The $12.5 million budget of the division, averaging out to $367,000 per staff member, not including other agency equipment funds, is as good as, or even better than, that found in first-class high-technology companies. The major portion of the budget is for scientific and technical research activities for NIST and other agencies of the U.S. government, showing the scientific importance of the division's work. About one-third of the portfolio is dedicated to programs related to public safety, security, and standards, showing the commitment of the division to one of the most important goals of NIST. Division staff identified no complaints about the lack of personnel, budget, equipment, or space to carry out projects. Therefore, this is a well-supported division with no obvious deficiencies in infrastructure.

OBJECTIVES AND IMPACT

The general goal of the SMSD is to serve the nation in areas of chemical metrology, research, standards, and data. The specific goals are to characterize the spatial and temporal distribution of chemical species and to improve the accuracy, precision, sensitivity, selectivity, and applicability of surface, interface, microanalysis, and advanced isotope-measurement techniques. The division carries various activities in order to accomplish these goals satisfactorily. Its work in chemistry metrology includes the detection of trace narcotics, the development of drug-delivery systems, the determination of molecular-orbital structure, and the electronic structure of organic electronics. Its research activities include the adsorption of self-assembled monolayers of nonspecific proteins, spectrometry using supercontinuum sources, the imaging of surface potentials of organic thin-film transistors, the transfer of quantum dots in an invertebrate food web, and super-resolution optical microscopy. Its work in standards development includes the preparation of polymer microspheres containing explosives, precision measurements of isotope ratios, and chemical mapping. Its data activities include reinvention of the Desk Top Spectrum Analyzer and the x-ray spectral imaging of cracks in bridges.

This work has demonstrated that the objectives of the division are being fulfilled successfully owing to the effort of its dedicated staff and the availability of the state-of-the-art equipment. The results can be anticipated to have major impacts on national security, the overall mission of NIST, and the scientific community.

CONCLUSIONS

The Surface and Microanalysis Science Division has successfully accomplished its own targets as well as those of NIST in serving the nation in areas of chemical metrology, research, standards, and data. Many of the scientific studies of the SMSD have achieved excellent results that have, for example, enhanced the capability to characterize surfaces and interfaces with increased accuracy and precision. The division has a competent technical staff with state-of-the-art equipment, advanced facilities, and sufficient budget. To further enhance the capability of the division to achieve its objectives and have more impact on the scientific community, those involved may wish to consider ways of expanding the division's collaborations with universities and national laboratories so as to make better use of its facilities and bring in fresh ideas as well as initiate explorations in new areas. Another path to improving the division's effectiveness is to bring in more theoretical experts, both within NIST and externally, for more in-depth interpretation of some of SMSD's excellent experimental data. A further area of possible improvement for some projects is a better definition of strategy, such as the long-term direction of scientific study and technology development. Since this division includes a wide range of activities, the development of a division-wide strategy could lead to greatly enhanced visibility and impact in the government and scientific communities.

7

Thermophysical Properties Division

SUMMARY

The Thermophysical Properties Division (TPD) is an outstanding service center. Its services are supported by research and by methodology development, and the equipment being developed is state of the art. Each group is running "mean and lean," and despite the small numbers of scientists in each group, the division is highly productive. The division seems to be a model of cost-effectiveness. The precision of the critical measurements, their incorporation into mathematical models and equations of state, and their availability through online databases have been and will continue to be highly valuable to industry, academia, and other government laboratories.

RESPONSE TO RECOMMENDATIONS FROM THE PREVIOUS REPORT

The Thermophysical Properties Division has made good progress in holding interdivisional seminars and promoting the cross-fertilization of ideas within the division. It has also increased efforts to coordinate the programming aspects of databases with other divisions, but more effort is merited in this area.

There has been a laboratory-wide effort to address the merits of patenting and licensing. In addition, the copywriting and licensing of access to databases should be considered, both as a means of increasing the dissemination of data and as a fund-raising activity. An effort has been made to increase the ratio of technicians to professionals, but the correct balance requires continued evaluation. Adequate laboratory space also remains an issue. Renewed efforts should be made to form an awards committee to seek out awards for researchers. Efforts are being made to help staff develop a good idea of the overall TPD mission as well as their own personal objectives.

Other divisions besides the TPD are also developing databases, and the coordination of the information technology aspects of these efforts should be expanded.

TECHNICAL MERIT

The Thermophysical Properties Division is composed of 3 groups (Thermodynamics Research Center Group, Experimental Properties of Fluids Group, and Theory and Modeling of Fluids Group) and 2 projects (Cryogenic Technologies project and Properties for Process Separations project). The FY 2008 TPD budget was approximately $7.8 million, of which approximately 71 percent was direct appropriation, 23 percent was other-government-agency funding, and 6 percent was measurement services funding. The staffing level is approximately 30 NIST FTEs, 7 visiting scientists, and 42 students, postdocs, and contractors.

The division's stated mission is to provide the best available measurements, theory, computations, and data evaluation for the thermophysical property information required to enable the development of standards, enhance productivity, facilitate trade, ensure scientific and technological progress, and improve the quality of life. To accomplish this, the division pursues a program of experimental measurement, data collection and evaluation, development of theoretically based models, and simulation of model systems, and its outputs include computerized standard reference databases that synthesize thermophysical property information in forms that are convenient for its stakeholders.

Program areas within the division include the following: energy (thermophysical properties, data, cryogenic flow, alternative fuels, aviation fuels, advanced power cycles); environment and climate (cryocoolers for Earth monitoring, properties for aerosol formers, carbon dioxide separations in power cycles, carbon dioxide emissions); bioscience and health (information infrastructure for biothermodynamic data, terahertz imaging with biological applications, standards for biocalorimetry); public safety and security (data for the identification and detection of explosives and taggants, cryocoolers for special applications); and standards (dynamic data evaluation, wide-ranging properties, information exchange, international equation of state for fuel gases, SRMs [density and viscosity]).

The Experimental Properties of Fluids Group of the Thermophysical Properties Division has developed a one-of-a-kind densitometer that provides valuable data that can help in determining the phase behavior of a range of fluids. This group has a strong interaction with the Theory and Modeling of Fluids Group, and there is excellent synergy between these two groups.

The techniques developed by the Properties for Process Separations project are state of the art. In particular, the group has developed a novel distillation apparatus that allows it to analyze carefully the composition of a range of complex fluids. The level of information that the group can thus obtain on industrially important liquids and gases is very impressive. The work on the volatile gases has importance for homeland security, and in this capacity the group is also providing a useful service that is highly timely and can ultimately be extended to a range of industrial applications (e.g., detecting the spoilage of food). The group is highly productive, with just a small number of researchers. There is good synergy with the theory group.

The work of the Thermodynamics Research Center is impressive—in particular, its development of a global information system for thermodynamic data is an important achievement and represents significant advances in computer science and data management. The code is not only an invaluable tool for researchers, but it also provides an excellent teaching tool. The group is working on the complicated issue of making this code available to the public in such a way that it could be used extensively but at the same time would help the group recover some of the development costs.

One of the strengths of the Theory and Modeling of Fluids Group is its strong interactions with all of the experimental groups in the division. The collaborative atmosphere is very apparent, and it is clear that both the theory and experimental groups benefit from these interactions. In particular, certain theoretical calculations are suggested to the Theory and Modeling of Fluids Group by the experimentalists, and the experimental studies are facilitated by input from the theory group undertaken on the basis of that input. The collaborations seem highly fruitful, and the people seem genuinely enthusiastic about the exchange between theory and experiment. The Theory and Modeling of Fluids Group is also involved with hosting the important Symposium on Thermophysical Properties, which is the oldest and largest conference in this area and further extends the outreach activities of this group. Also with respect to outreach, the group maintains and updates a database (Reference Fluid Thermodynamic and Transport Properties Database, REFPROP) that is a valuable tool for obtaining data about the properties of fluids; this is also a useful teaching tool. The group does a commendable job of providing service to the scientific community.

The activities of the Cryogenic Technologies project group also reflect the role of NIST in designing state-of-the-art equipment that is playing a vital role. The cryogenic-flow calibration facility is unique, as is the expertise provided by the small but highly productive group. Its knowledge base will be invaluable for expanding the hydrogen economy and the nation's further use of liquid natural gas.

In FY 2007, division researchers produced 47 publications and gave 65 talks (including 8 posters). In FY 2008, division researchers produced 50 publications and gave 103 talks (including 5 posters). Seventeen division staff members are credited with currently and/or recently holding professional committee assignments and 10 with holding editorship positions.

INRASTRUCTURE

The Thermophysical Properties Division is currently cramped for space. This problem is expected to be eased by the addition of the new building under construction.

EXTERNAL INTERACTIONS

Most groups within the Chemical Science and Technology Laboratory have substantial interactions with others working in the field, including visiting scientists from other government laboratories, industry, and universities. In addition, they have collaborative interactions with industry groups, university consortia, and joint efforts with other government laboratories. Such associations aid them in determining valid long-term goals and allow them to benefit from new technology being developed outside the CSTL. These are powerful incentives to seek the right blend of such associations. Too much direct service work, while bringing in additional funds, could dilute longer-term strategic work on new technology to support the TPD's mission. Associations and collaborations with industry are particularly valuable, since they help focus the division's (and CSTL's) activities in new technological directions that are being driven by the marketplace. Since one of NIST's overall goals is to support and nurture the economy, cooperation with industry will help support such a goal. It is important, of course, to try to strike a balance between current industrial needs and new technology emerging from academia and other government laboratories.

One way in which the division might seek out more industrial input would be to join existing academic-industrial consortia in areas of interest. This would put them in contact with more industrial scientists and academics that have common interests. A number of such consortia have been successful in the catalysis and control/optimization areas. Of course, some of these consortia require paying for membership, but it might be money well spent. Many companies have efforts similar to those of the division, addressing specific materials that are critical to them. Interactions with such companies to share information could be beneficial to both the division and industry.

INFORMATION DISSEMINATION

The TPD is making a good effort to disseminate its information through publications, professional meetings, seminars, and industrial associations. It also recognizes the growing importance of establishing databases that are accessible through the Internet. While there is already a substantial effort in this area, it is such a critical activity for the division that this effort should be further strengthened. Commercial databases are also under consideration, and pilot activities to determine their value should continue. Industrial companies and trade associations also maintain databases in their areas of interest, and these should be evaluated. For example, ExxonMobil is developing a database for properties of thousands of hydrocarbons and petrochemicals, using a technique called structure-oriented lumping. It is possible that ExxonMobil might be willing to work with the division in this area.

OBJECTIVES AND IMPACT

The stated goals of the Thermophysical Properties Division are to determine the thermophysical properties of gases, liquids, and solids—both pure materials and mixtures, and fluid-based physical processes and systems, including separations, low-temperature refrigeration, and low-temperature heat transfer and flow.

In the area of thermophysics, the division develops, maintains, and uses state-of-the-art apparatuses to perform experimental measurements on industrially and scientifically important systems; compiles, evaluates, and correlates experimental data; develops and evaluates state-of-the-art theories, models, estimation methods, and computational approaches; and disseminates results by a wide variety of mechanisms.

In the area of cryogenic technologies, the division provides engineering data, models, and research to support the development of advanced cryocoolers; and measurement methods, tests, and calibration services for flow under cryogenic conditions.

The potential impacts of the success in the division's research areas are the precise characterization of complex fluids that are important for industrial applications; detailed thermodynamic information that is vital for fundamental studies on various fluids; a useful computational tool on thermodynamic data that can also be used as a teaching tool; and the expansion of the knowledge base invaluable for expanding the hydrogen economy and the nation's further use of liquid natural gas.

CONCLUSIONS

The panel's overall impression of the cost-effectiveness of the Thermophysical Properties Division was favorable. The division may wish to increase its efforts to measure its cost-effectiveness or research-to-return ratio by identifying the value of its work to its customers. The more customers can testify to the benefits derived from the division's products, the greater the creditability of the TPD's research-to-return ratio. The higher the creditability, the more likely it is that the division could justify more resources.