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National Science Foundation
Workshop on Chemistry and Sustainability

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Pacific Northwest National Laboratory
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Executive Summary

Sustainability: development that preserves the needs of the present without compromising the ability of future generations to meet their own needs.

-definition provided by Geoff Coates, co-chair of the National Science Foundation Workshop on Chemistry and Sustainability. (source: www.sustainablemeasures.com, accessed Sept. 27, 2005)

The National Science Foundation considers sustainability an important area for the mathematical and physical sciences, and the Foundation's chemistry division is contemplating placing emphasis on sustainability research. Twenty-six early career chemists and chemical engineers participated in the Foundation's "Workshop on Chemistry and Sustainability," November 3-4, 2005, at the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. Participants discussed the most important challenges currently facing chemistry and sustainability at the molecular level within and between the four elements: earth (soil), wind (atmosphere), water, and fire (energy). More specifically, they considered the kind of research objectives that would support each area. While grand challenges are what motivate and drive research, smaller initiatives need to be addressed and solved within the context of each challenge.

Researchers were invited to participate in the workshop based on their area of expertise in chemistry. These scientists represented a variety of subdisciplines within chemistry. As the chemistry components of sustainability research arise from these distinct branches of the discipline, research initiatives need to be collaborative and cross these boundaries as well.

Branches, or subdisciplines, of chemistry represented at the workshop:

- Aquatic chemistry
- Atmospheric chemistry
- Energy production and storage
- Geochemistry
- Green chemistry/synthesis

Workshop participants shared some sobering statistics, which undoubtedly drive a great deal of sustainability research:

- Agriculture uses 40 percent of the U.S. water supply
- Cooling at power plants uses another 40 percent of the U.S. water supply

- 70 percent of all antibiotics in US are used on farms
- The human population expected to increase to 10 billion by 2050
- In 20 years, half of the world's population will live in water-restricted areas
- 150 million tons of plastics are produced worldwide each year
- About 10 percent of the oil we use every year goes into making plastics

The Grand Challenges are arranged around some very broad but important themes that drive sustainability and were frequently mentioned during discussions throughout the workshop. Those included:

- **Urban metabolism, or studying an urban area as a unique, contained ecosystem**
- **The effects of human activities on the environment, and in turn how an altered environment affects human health**
- **Cycling of materials and the resulting energy used and given off and waste that results**
- **Developing alternatives to fossil fuels**

Workshop Design

The workshop was designed around a series of four breakout sessions. Prior to the first breakout session, researchers introduced themselves, their research and three grand challenges they felt were important in driving chemistry-based sustainability research. The group as a whole was given several opportunities to discuss these challenges.

Participants were divided into one of five groups for each breakout session. In the first breakout session, groups were formed according to research interest – aquatic chemistry, atmospheric chemistry, energy production and storage, geochemistry or green chemistry. For example, all of the atmospheric chemists met as a group. The workshop organizers asked each group to come up with five to eight grand challenges facing that group's respective area of expertise. After this session, workshop participants reconvened and discussed the challenges the individual groups had outlined. (**SEE APPENDIX**)

For the second breakout session, participants in different chemistry subdisciplines met in groups (for example, an organic chemist and a geochemist may have been in the same group.) Again, the groups were asked to come up with five to eight grand challenges facing chemistry and sustainability, and a list of potential research objectives to support each challenge. (**SEE APPENDIX**)

During the third breakout session, participants were again split into five groups and asked to identify the science drivers and potential funding mechanisms for chemistry and sustainability initiatives. Afterward, the entire group reconvened, and representatives from each breakout group discussed their suggestions with the entire group.

During the fourth and final breakout session, the smaller groups were each assigned one of five grand challenges. These final challenges had evolved throughout the workshop, from the earlier presentations and discussions. Each group was asked to discuss ways to address these challenges. The final list of grand challenges is outlined below:

- Understanding transformations at interfaces
- Understanding both natural and human-induced cycling of the elements
- Catalysis: Diverse environments and applications
- Key targets for new characterization techniques
- Scaling up: Studying interfacial phenomena in terms of time and size scales

A thorough description of challenges and their respective objectives, along with a discussion of the funding mechanisms necessary to have in place for a successful sustainability research initiative, comprise the main body of this report.

The appendix, beginning on page 16, will show the reader how the grand challenges metamorphosed during the two-day workshop. It contains a thorough overview of the discussions that led up to the formation of the final grand challenges. The appendix begins by listing some of the grand challenges presented by individual investigators at the beginning of the workshop. Also included are the challenges and discussions resulting from the first and second breakout sessions.

The Grand Challenges

One participant related the grand challenges of sustainability to finding a cure for cancer, which is undoubtedly a grand challenge facing medicine. Many smaller initiatives, or drivers, need to be in place before any one of the challenges can be fully realized.

This section of the report explains the five grand challenges in detail and in the order they were presented at the workshop. These grand challenges are a culmination of the many challenges facing chemistry and sustainability that individual researchers and groups presented throughout the workshop. Workshop co-chairs Heather Allen and Geoff Coates drew up this final list from distillation of the grand challenges presented by the workshop participants. Included in the description of each challenge are the objectives supporting that challenge.

Understanding chemical transformations at interfaces

Chemists deal with heterogeneous, multiphase interfaces that have complexity layered on top of already complicated chemical transformations. It is critical to understand these transformations at the molecular level, and across boundaries such as at the interface between air and water, water and soil and soil and air. Understanding chemical transformations at interfaces may also provide a better understanding of catalysis, natural and designed catalytic systems.

Research supporting a better understanding of the chemical transformations at and across interfaces includes learning how:

- aerosols and clouds form;
- aerosols transport pollutants, and what happens as aerosols degrade;
- aerosol degradation/transformation affects climate;
- to reclaim, recycle and manage waste water;
- pollutants are transported by water;
- weathering and erosion affect soil quality, including the effects of mining on soil quality;
- landfills function: landfills are a depository, but they can also leach pollutants through soil and water; and

- how to convert solar energy to electricity (storage issues).

One issue addressed often during the workshop was the problem of finding alternative fuel sources, or feedstocks, to replace fossil fuels. Energy production and use are both controlled by chemical transformations, so it is imperative to understand the interfacial transformations needed to convert feedstocks into usable fuel sources. And as one participant pointed out, figuring out how to store energy, and reduce the cost of that storage, is critical if scientists are to develop new energy solutions.

This group also pointed out that it is necessary to confront our society's disposable culture with a better understanding of how synthetic materials break down and interact on the molecular level at water, soil and air interfaces. Considering the energy associated with producing, using and disposing of the materials that contain the chemicals in those synthetic materials is key.

Upon hearing the presentation, one workshop participant asked that if it's not possible to make products that are recyclable, maybe it is possible to design products that are biodegradable.

Understand natural and human-induced chemical cycling of the elements

Scientists must understand and be able to control and optimize the flow of matter and energy. Key to this challenge is closing the "loop of usage" on chemical transformations. Energy is consumed and produced throughout an object's life, whether it is a cell phone or a child's toy. This loop of usage has three main components: production, use and disposal. Human activity is an integral part of each component. One goal is to minimize resource depletion caused by manufacturing new materials, which would theoretically help minimize the pollution produced when the material is disposed. Another goal is to find ways to contain the energy produced when an object is broken down.

Objectives supporting this grand challenge:

- Life-cycle analysis
    - Every material, whether natural or synthetic, has a defined life cycle; scientists need to be able to predict beforehand the effect that a particular material has on the environment throughout its life cycle

    - Scientists need models to understand life-cycle analysis at various interfaces, yet very few researchers do the necessary molecular-scale computations for this kind of long-term analysis

    - Develop new processes for breaking down existing materials (one suggestion: it may be possible to use lactic acid to break down polymeric materials)

- Develop fossil fuel alternatives
    - Address how changes in energy sources, or feedstocks, affect the environment

    - Identify, develop and use renewable feedstocks (such as polylactide and from carbohydrates) that can replace fossil fuels

    - Tailor the properties of those feedstocks so they can be the most efficient fuel sources possible

- Use waste as a feedstock
    - Figure out how to separate complex mixtures, such as the components of a personal computer

    - Find ways to recover the chemical energy given off by the production, use and disposal or breakdown of a product

    - Support efficient conversion of waste to fuel sources

Catalysis: Diverse environments and applications

Catalysis is a dynamic process that modifies and increases the rate of a reaction. The catalyst is not consumed in the process. Here lies the challenge of designing different, more efficient and environmentally friendly catalysts, and understanding how those catalysts behave at the molecular level (interfacial catalysis.) The catalysis group further explained their challenge by breaking it down into five central themes, or drivers, that characterize catalysis at environmental interfaces, which are constantly changing. Four of the themes are organized around molecular mechanisms, a fundamental part of all interactions. One workshop participant expressed that to study sustainability means to ultimately understand the molecular mechanism for everything chemists observe.

Reactions at environmental interfaces and the molecular mechanisms that control those interfacial reactions drive catalysis research. These interactions include all elements – earth, air, wind and fire – and happen between all of the elements. Examples include aerosols and clouds;

colloidal surfaces (such as the interface between the ocean surface and the atmosphere); and even biofilms (such as the water-repellant skin on a duck.)

Objectives that support the catalysis challenge:

- Use chemical synthesis to make new catalysts
    - Develop and identify eco-friendly feedstocks from non-precious metal catalysts and biorenewable agents (such as oxygen, nitrogen, carbon dioxide and biomass)
    - Consider different kinds of reactions that could be used for catalysis, such as oxidations, reductions and biocatalysis
    - Develop "green" processes by which to do this (for example, use techniques such as green media, tandem reactions and by-product minimization)
- Energy production and storage
    - Develop fuel cells that act as electrocatalysts
    - Capture solar energy and use it to create energy, a process called photocatalysis. Also, use photocatalysis to produce hydrogen
    - Learn the best ways to store and transport energy (batteries and superconductors)
- Remediation and recycling may benefit from advances in catalysis
    - Wastewater treatment and reuse
        - Use catalytic disinfection agents to treat water to make it reusable
        - Figure out how to reuse wastewater for industrial cooling
        - Understand the chemical transformations that occur during treatment
        - Develop membranes that can help facilitate treatment and reuse
    - Air-gas (atmospheric) treatment
        - Build better, more efficient catalytic converters
        - Understand what kind of interfacial interactions are happening in the atmosphere, such as the life cycle of aerosols
        - Develop ways to catalytically remove contaminants in a smokestack
    - Treating toxic soil
        - Toxins come from a variety of sources, such as the drainage from mining and toxic waste sites
    - Chemical processing to facilitate more efficient remediation and recycling

- Can safer catalysts be used or developed for these processes?
- Learn what mechanisms would make these safer catalysts usable

Key Targets for new characterization techniques

Particles in the air, water and earth and in catalytic reactors are complex entities that are difficult to describe because they comprise multiple phases, mixing states, morphologies and layers. Therefore, it is necessary to have detailed structural characterizations of the organic compounds that are associated with these extremely complex biological and chemical particles. Knowing how these particles behave and act at various interfaces will lead to a better understanding of how they affect environmental and human health. Such understanding could help scientists detect environmental toxins and biological threats. The composition of nanoparticles is extremely important to understand, as their size and composition can affect chemical reactivity, climate change, nucleation and human health. Ideally, the technology allowing this kind of observation is inexpensive in order to facilitate its widespread distribution.

With the proper support, scientists can develop low-cost sensors and purification strategies, along with techniques that can measure all of these components at the same time, given that interfaces continuously change and that there are also may components functioning on any given interface.

Such instrumentation and techniques would allow scientists to quantify simultaneously, and in some cases at lower concentrations, all of the ions and other substances (and in other forms) in water, including nitrate, phosphate, mercury, arsenic and chromium, which all have an adverse effect on the environment. Techniques to facilitate interfacial separations are also key; such techniques could address pathogen removal, the use of catalysts in byproduct removal, alternatives to chromatography and developing alternative extraction solvents to avoid water contamination.

This group provided a list of the ideal characteristics for instrumentation that would allow scientists to characterize interactions at the interface:

- Miniaturization, perhaps through lab-on-a-chip technologies;

- high sample throughput;
- small sample size;
- portable for field work;
- real time analysis in remote locations;
- remote sensing capabilities;
- three-dimensional spatial and temporal reporting capabilities;
- remote sample analysis to expedite research;
- robust sensors that report detailed chemical information at high temperature and pressure conditions (e.g. for catalytic reactors);
- selective sensing of trace components in the presence of large amounts of interfering compounds; and
- methods that possess a large dynamic range.

Scaling up: Studying interfacial phenomena

Interfacial interactions happen on all levels, from the molecular to the global. Scientists need to think of these interactions in terms of time scales and size scales. This group challenged workshop participants to "link laboratory observations with predictive models to build molecular-level frameworks for predicting the impact of human activities on the environment." But such models are needed before the fact, before the proposed interaction actually happens. Models provide the feedback that guides new experiments to further the understanding of these multiple-level interactions. At the urban and global levels, pollutants cross interfaces and react in different ways based on a variety of criteria, including weather, climate and the pollutant's age.

Molecular-scale simulations, molecular-based frameworks and descriptions, all are necessary to understand and predict interfacial interactions. These models work across chemistry disciplines, too: atmospheric chemistry, biochemistry and geochemistry. The group provided watersheds as an example of a contained, dynamic environment that could benefit from multi-scale modeling research. It suggested a refocus for aquatic chemistry, such as identifying the source of contaminants and modeling their removal.

Predictive models may also work for understanding how shifting from a fossil-fuel economy to another fuel source or feedstock changes the atmosphere, and ultimately the climate. Finally, scientists need to agree about what kind of time scale they are working on, as all of the grand challenges are long-term issues, requiring long-term problem solving initiatives.

Mechanisms of Funding

While funding mechanisms were discussed separately from the final list of grand challenges, how to fund sustainability research presents a unique challenge. As there are currently no well-defined programs in place to fund sustainability endeavors, the National Science Foundation asked workshop participants to brainstorm and discuss creative ways to fund such initiatives, ones that would provide an opportunity for science and sustainability research to move forward. Participants were also asked how current funding structures could change to encompass the long-term visions that address multi-scale sustainability problems.

Potential ways to fund sustainability research initiatives:

- ***Grants***

Provide grants for multi-investigator proposals. For example, fund groups of any where from two to five principal investigators. Ensure that these grant recipients can meet face-to-face annually to collaborate. These grants should be funded at or above the single-PI grant level. Ensure that they are restriction-free for participants, universities and institutes. Collaborative research is typically more time-intensive than single PI research for each PI. Therefore, ensuring that there are a significant number of these grants available is critical for encouraging investigators to pursue collaborative research.

Seed grants for young researchers can fund a greater number of scientists than can traditional full-scale grants. Seed grants also foster more competition, which in turn encourages and benefits sustainability research. Offer a significant number of seed grants at the junior and senior faculty level. As a way to entice the involvement of industry as well as leverage NSF dollars, the NSF could offer matching funds (i.e. dollar for dollar) for any seed grantees who successfully engage industry and obtain funding.

Funding must be long-term, as sustainability issues may last for years.

- ***Create decentralized centers***

Attract bright young researchers and help level the playing field for younger principal investigators by establishing decentralized research centers. Create sustainability-focused centers at two or three universities around the country, with combined funding from multiple sources, including the Department of Energy, NSF, the National Institutes of Health, etc. The NSF could also coordinate and oversee consortia of academic and industrial interests.

Such centers could be comprised of small group projects, led by a project team of two to four single PIs. Again, the researchers involved must be given the opportunity to meet annually. Inviting industry and non-governmental interests to these collaborative meetings would help ensure that the PIs keep a real-world focus on their research objectives. Collaborating with industry may also be a way to foster a decentralized focus, although industry may demand first patent rights to any technology coming out of the collaboration.

Several individuals stated concerns over university- and department-based centers continuing the already established research of senior PIs and thus creating a culture of the "haves and have nots". The workshop attendees did not view this cultural norm in a positive or collegial light. However, there was some disagreement on the types of centers -- and which centers -- that this culture developed.

- ***Other modes of funding sustainability research***

Establish programs within NSF's Collaborative Research in Chemistry (CRC) program to fund a sustainability ('sus')-in-chemistry initiative. This initiative could fund a 'Sus' postdoctoral fellowship program. Create a 'Sus' directorate in the CRC; the directorate could serve as a funding model. This 'sus' initiative could drive collaborative research on single PI grants. Creating the next generation of professors in the area of sustainability was also addressed and deemed critically important; this is an area in which the Sustainability Postdoctoral Fellowship could make a positive impact.

Researchers need the money to acquire the equipment and develop the techniques necessary for pursuing sustainability research endeavors. Also, makers of the equipment and techniques ideally will be in the same room as those who are using the tools to measure interfacial reactions, molecular mechanisms, etc. Technology centers, such as PNNL, need to allow access to this specialized equipment. Such centralized facilities can offer better computational resources, more efficient algorithms and also have the capability of handling large datasets.

Offer additional funds for travel to collaborative meetings (such as a workshop) or offer non-competitive bonus money on top of single PI grant in order to foster collaborations.

- ***Measuring the success of funding programs***

  - Academically: through publications and the number of masters and doctoral students graduated

  - Real-world: through patents granted, processes and policies adopted by industry or government and environmental assessments

  - A problem with the current system is that it has reviewers who are narrowly focused on defined areas of expertise, instead of viewing problems holistically

- ***Educating the public***

Offer specific funds for educational and outreach components, which are distinct from the specific proposal. Accomplish three to four outreach activities during a funding cycle

Provide international grants for collaborative efforts between developed and developing countries. The developed nation would fund these grants.

- ***The challenge of funding sustainability initiatives***

Funding for sustainability projects needs to be long-term and stable and determined by the context of the research, not solely by the discipline. This approach to funding naturally fosters a multidisciplinary approach. Also important is having enough flexibility to re-align funding if the funder or the grant recipient sees that the project is ultimately going in a different, yet viable direction.

Conclusions

There are important opportunities for the chemical sciences to contribute to a better understanding of the environment through sustainability research. The grand challenges represent some of the key issues facing chemistry and sustainability. Workshops like this one that nurture cross-disciplinary collaboration are critical, as they begin to foster that sense of community across disciplines. The NSF and the participants in the Workshop on Chemistry and Sustainability realize that it's time to refocus the thinking of the broader scientific community, and that involves bringing together scientists from different disciplines. Such action represents a cultural shift in the scientific community, and as such will take great effort to maintain and to see through to a successful end result.

Appendix

The appendix contains grand challenge themes that emerged throughout the workshop prior to the last breakout session when participants were asked to address a specific set of challenges. Those five final challenges evolved from previous discussions during the workshop. Summaries of those discussions are highlighted here, to give the reader insight into the evolution of these challenges.

Individual presentations
Before the first breakout session, each researcher shared with the group what he or she felt were the most important challenges facing chemistry and sustainability. Some of those challenges included:

Urban metabolism: studying urban environments as closed systems
Cities are contained, sustained organisms with numerous interactions that are constantly happening. These interactions range in scale from the molecular level to the multi-interface level, and as such affect the urban environment internally as well as externally. Changes in growth patterns, such as urban sprawl, ultimately impact air, water and soil quality.

Human health and human influence on the environment
Interactions at environmental interfaces affect human health – pollutants are transported through soil, air and water and aerosols form and degrade in the atmosphere. These interactions affect our drinking water, the air we breathe and the farmland that supports crops. And much of the interfacial activity at the molecular level can be traced back to some human activity.

Clean air and a better understanding of aerosols
The reaction kinetics of aerosols are poorly understood, and interactions with pollutants can increase the life span of many aerosols. It's also important to be able to separate naturally induced changes from changes caused by humans.

Some of the other challenges facing aerosol research include:

- Learning where aerosols come from and how they form, along with their role in cloud formation
- Understanding the reactions of organic matter in aerosols and how these reactions affect climate
- Understanding these processes at the molecular level
- Studying the role of biological materials in atmospheric aerosols
- Learning what can be down to reduce the presence of aerosols
- Understanding how solar energy drives chemical reactions in the atmosphere

Catalysis
Scientists need to develop more efficient, environmentally sound catalysts to drive important reactions, such as creating energy as well as catalysts that can speed up processes of remediation. There needs to be in place catalysts that support a mix of alternative energy sources; this is especially important in order to support a steadily growing global population.

Other challenges facing catalysis research:

- Their synthesis needs to be benign
- Possibly use microwave technology as an inexpensive and benign way to heat up and speed up reactions
- Develop improved electrocatalysts for fuel cells, because we need low-cost, efficient new catalysts for fuel cell applications
- Consider using photoactive materials, which are more energy efficient, for catalysis; these contain a lot of energy that could be used to drive reactions

Cycling of materials and nutrients (production, consumption, disposal)

Complete sustainability establishes a circular flow of materials. In an ideal world, all materials would be fabricated from renewable resources and, therefore, eligible for bioremediation or recycling at the end of their lifetime. Energy is used and produced throughout an object's life cycle – is there a way to harness this energy?

Challenges facing the study of recycling and reducing:

- Separate complex mixtures – for example, consumer electronics – and convert the components of these products into useful precursors for new materials
- Depend more on renewable resources to provide raw materials
- Make polycarbonates completely from renewable resources
- Start with benign materials
- Determining how renewable and recyclable materials will be used will help to minimize waste streams

Predictive modeling

Most modeling is reactionary – it's done in response to an observation. But modeling is also a useful tool for studying current changes and for predicting what could change based on any number or type of interaction. Examples include measuring how much carbon dioxide a city – a closed urban environment – would emit based on changes within the city, such as new transportation infrastructure and the building of new neighborhoods.

Finding new energy sources, then producing, storing and using those sources

Key here is reducing our global dependence on non-renewable resources. Although it's a tall order, scientists must find and/or develop and use renewable energy resources that aren't petroleum based and won't damage the environment.

There is great debate over whether a hydrogen economy is truly the way to go. Right now, hydrogen production is fueled by fossil fuels. Also, shifting to a hydrogen economy will undeniably change the makeup of the atmosphere.

Challenges facing energy research initiatives:

- How to store large-scale amounts of renewable energy and electricity
- Determine if biomass is a renewable energy source
- Establish independence from carbon with renewable carbon-free energy sources

- Scientists need to learn if large-scale sustainable production of hydrogen without fossil fuels is even possible
- What issues surround the transition to a hydrogen economy? Issues include those of transportation, storage and safety
- Develop efficient technologies for solar energy collection. Politically, the time is right to move toward solar energy, but the area needs more research and investment

Ensuring clean, plentiful water supplies locally and globally
One key here is improving technologies for treating and reusing water and wastewater. But these purification techniques need to be cheap, so they can be widely distributed.

Also, the proper models can address what happens to water at the surface, at the interfaces.

Techniques and instrumentation
Scientists need continued support to keep developing aerosol mass spectrometric techniques – techniques that can characterize the structure, mixing state and surface composition of real aerosols. New techniques and tool will also help researchers develop new, readily accessible materials that are potentially biodegradable or recyclable.

Collaboration and multidisciplinary efforts
The Workshop on Chemistry and Sustainability represents an early effort to combine the expertise of subdisciplines. The NSF, and the participants involved in the workshop, recognize a need for interdisciplinary approaches to solving sustainability issues.

Education and outreach – best ways to communicate sustainability science
Public opinion is based on public perception. It's the scientist's job to ensure that the public buys into the opinion that sustainability research efforts are a worthy cause. The public includes business, industry, politicians, funding agencies, taxpayers, and so on. It's also important to educate end users – those who would use the technology that these research efforts develop. For example, it may be difficult to encourage a rural village in Africa to use electricity-carrying wires coming out of a black box on a pole, when the village has been using much more primitive methods for energy production for generations. Another example are urban and city planners – those whose decisions are most likely to affect urban metabolism at all levels, from the molecular, internal to the boundary-crossing (the boundary between the urban environment and the countryside on the other side of the bound, for example)

Grand Challenges presented after the first breakout session

Once the individual presentations were finished, participants gathered into five smaller groups for the first breakout session. In this round of breakout sessions participants in each group roughly represented expertise in one of five key areas -- aquatic chemistry; atmospheric chemistry; energy production and storage; fossil fuels; and green chemistry. Each group was asked to come up with five to eight grand challenges within their area of expertise.

Challenges described following this round of breakout sessions included:

Improving water quality
Understanding molecular-level chemical transformations, or the interfacial chemistry going on between molecular surfaces, is one key to improving water quality. Researchers need to have tools to characterize water quality, such as cheap sensors that can measure individual interfacial reactions, instead of relying on aggregate measurements. Tools that identify emerging contaminants, such as pharmaceuticals, perchlorate and NDMA (N-nitrosodimethylamine) are also necessary.

Globally, we are being forced to rely more and more on lower quality, which is leading to higher levels of treatment. But is it possible to find the source of all of the different components that pollute water? We don't want to be in a state of constant remediation – that's expensive. Also, what are the processes that affect water quality in natural and man-made systems?

Collaboration
More cross-disciplinary interaction is needed between standard disciplines to fuel sustainability research

Prime sources of oxidation are from paper and laundry bleaching (Stahl)
We can't get rid of waste; we produce it daily
How to kill pathogens

Political issues
What methods of energy production, use and storage are most likely to be implemented in third world countries? Also, conduct research in the context of (knowing that there are) all of the political issues surrounding access to clean water.

Energy – alternative sources; production, use and storage
The global population is booming, and promises to continue growing. There needs to be enough energy to meet future demands. Chemists can solve the issues these demands present – issues of energy production, storage and use. Energy storage is a problem of capacity, and the chosen storage systems need to be transportable.

Once scientists find alternative fuels, or feedstocks, they need to know how to sustain the high-caloric energy feedstocks

Solar energy is a promising source, but the scientific community needs more support to study the possibilities of solar energy. For one, photosynthetic processes may be a source of creating biomass to make a new fuel source. Is it possible to use photosynthesis to grow biofuels?

Modeling/scaling up
Take a holistic approach to scaling up: make molecular-level models of the events that happen at interfaces, along with macro-scale models of events that happen on the urban and even global level. Understanding molecular-level principles of interactions, fostered by this capacity/ability

to scale up encourages more efficient science. Unlocking the mysteries of molecular-level differences could help predict, and perhaps prevent, undesirable outcomes. Modeling pushes scientists toward studying real-world systems.

Atmospheric quality and human health

Most of the discussion about atmosphere centered around humans – the effect of human activities on the atmosphere and, in turn, the health effects caused by the treatment of heavy metals and pesticides. That is, how do these pollutants in their gaseous phases affect human health? And how do these pollutants change once they mingle with other particles in the atmosphere?

Aerosols undoubtedly change atmospheric quality, therefore it's necessary to understand the interfacial chemistry of aerosol surfaces. Scientists also need to know at what concentration a pollutant becomes a pollutant, and if there is a level that humans can tolerate before truly calling a pollutant an environmental or atmospheric contaminant.

Results from this kind of research may help to reduce the effects of human activities on climate.

Green chemistry/catalysis

Green chemistry methods are benign and produce little to no pollution. It may be possible to use green chemistry methods to develop renewable feedstock materials, as well as minimize the wasteful output of synthetic processes. An example of green chemistry is using green media, such as water, to facilitate reactions, rather than using toxic solvents.

Another goal is to speed up catalyst develop by decades and to predict the life cycle of a catalyst

Grand Challenges presented after the second breakout session

During the second round of breakout sessions, participants from different subdisciplines were placed into the same groups, and again asked to develop five to eight grand challenges based on previous grand challenge-related discussions during the workshop. Many groups noted a definite interface between the different researcher interests within groups.

Challenges resulting from this round of breakout sessions included:

Using scales to understand complex interfaces

Adopt a multi-dimensional way of thinking about environmental sustainability, and use predictive modeling to understand what could happen at interfaces at different points in time.
Understand the biological interactions at important interfacial processes
It requires understanding chemical interfaces by using models and multiphase systems. One workshop participant asked that if scientists can understand something that's going on at the interface in soil, which is a very complex environment, can they also take that knowledge and use it to figure out how to make catalysts that resist poisoning. And can scientists also develop

very complex custom catalysts for specific tasks or catalysts for dynamic environments where the conditions for the chemical species that are present are always changing.

One thing is certain – change is constant at all interfaces

Develop specialized "smart" sensors

These smart sensors can detect the differences at interfaces, and they also resist fouling, damage and corruption. Rather than being passive, such sensors could determine what kind of remedial action should be taken to reduce the propensity of environmental contaminants, whether in water, on the land or in the atmosphere. Their (remote sensing) feedback could lead to corrective action

Reduce usage and waste

We can't avoid usage on any level, whether industrial, commercial or personal, but we can reduce usage. For example, more efficient catalytic processes could help reduce the temperature at which industrial cooling reactions are currently conducted

- No choice but to build better purification methods.
- Develop advanced purification techniques
- Reduce dependence on precious metals and water
- Develop "super bugs" that can facilitate recycling and remediation

Water is the solvent of life. Our job is to rethink its biological kinetics

- Develop more advanced, smarter ways to purify water
- First need to figure out what in/about water should be purified – what is in there that is unsustainable?

Collaboration

- Pair chemists from different disciplines within chemistry to come up with a better system for sustainability research
- These experts need to collaborate with each other, and have the funding to support these collaborations
- Overcome the language barrier between disciplines and subdisciplines (for example, a word like 'sustainability' may mean something entirely different to a synthetic chemist than to geochemist)

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Workshop Agenda

Wednesday, November 2, 2005

12:00 – 10:00 pm	Check in at The Guest House at PNNL, 620 Battelle Blvd. Richland, WA 99352 (Phone: 509-372-6736). After hours check in instructions at the main entrance.
7:00 – 9:00 pm	Wine and cheese reception, The Guest House at PNNL, Suite 1130.

Thursday, November 3, 2005 (EMSL, Room 1075/1077)

7:30 – 8:25 am	Badging, Breakfast and Introductions
8:25 – 8:30 am	Welcoming Remarks: PNNL
8:30 – 8:45 am	Overview and Charge: Geoff Coates and Heather Allen
8:45 – 9:15 am	Six speakers, 5 minutes each: overview of research and 3 Grand Challenges: Crist, Stevenson, Bernhard, Criscenti, McNeill, Coates
9:15 – 9:30 am	Discussion of Grand Challenges
9:30 – 10:00 am	Break and Refreshments
10:00 – 10:15 am	Workshop Context: NSF (Videolink)
10:15 – 10:45 am	Six speakers, 5 minutes each: overview of research and 3 Grand Challenges: Allen, Blackwell, Noziere, Woods, Lee, Stahl
10:45 – 11:00 am	Discussion of Grand Challenges
11:00 – 11:30 am	Six speakers, 5 minutes each: overview of research and 3 Grand Challenges: Foster, Sanford, Mainardi, Roeselova, Weck, Martinez
11:30 – 11:45 am	Discussion of Grand Challenges
11:45 – 1:10 pm	Working Lunch (Allen/Coates to present overview of Grand Challenges from first two sessions, Discussion)
1:10 – 1:30 pm	Four speakers, 5 minutes each: overview of research and 3 Grand Challenges: Chirik, Nelson, Rosso, van de Krol
1:30 – 1:45 pm	Discussion of Grand Challenges
1:45 – 2:05 pm	Four speakers, 5 minutes each: overview of research and 3 Grand Challenges: Francis, Chellam, Geiger, Barney
2:05 – 2:20 pm	Discussion of Grand Challenges
2:20 – 2:30 pm	Overview of Charge and Explanation of 1st Breakout Session
2:30 – 3:00 pm	Break and Refreshments
3:00 – 4:30 pm	Break-out session 1: Identify 5-8 Grand Challenges

Red 1	Orange 1	Yellow 1	Green 1	Blue 1
Geiger	McNeill	Stevenson	Francis	Crist
Blackwell	Chellam	Bernhard	Chirik	Lee
Martinez	Nelson	Mainardi	Stahl	Noziere
Criscenti	Woods	van de Krol	Sanford	Roeselova
Rosso	Allen	Coates	Weck	Barney
				Foster

4:30 – 4:45 pm Break

4:45 – 6:00 pm Breakout session presentations and Group Discussion to identify 5-8 Grand Challenges, Summation

6:00 – 7:00 pm Free time

7:00 – 8:00 pm Dinner, Dr. Bills Bistro, EMSL

8:00 – 11:00 pm Informal discussions, wine and cheese reception, The Guest House at PNNL, Suite 1130

Friday, November 4, 2005 (EMSL, Room 1075/1077)

8:00 – 8:50 am Breakfast

8:50 – 9:00 am Overview of Breakout Session Charge: Grand Challenges

9:00 – 10:00 am Break-out session 2: Identify 5-8 Grand Challenges

Red 2	Orange 2	Yellow 2	Green 2	Blue 2
Noziere	Barney	Roeselova	Lee	Crist
Stahl	Weck	Sanford	Chirik	Francis
Martinez	Rosso	Criscenti	Blackwell	Geiger
Mainardi	Foster	van de Krol	Bernhard	Stevenson
Nelson		Woods	Chellam	McNeill

10:00 – 10:15 am Break and Refreshments

10:15 – 10:45 am Breakout session presentations and Group Discussion to identify 5-8 Grand Challenges, Summation

10:45 – 10:50 am Overview of Breakout Session Charge: Science Drivers, Tools, Funding Mechanisms (Collaborative Grants, etc.)

10:50 – 11:50 am Break-out Session 3

Red 3	Orange 3	Yellow 3	Green 3	Blue 3
Roeselova	Lee	Noziere	Barney	Foster
Stahl	Francis	Chirik	Sanford	Weck
Blackwell	Rosso	Geiger	Martinez	Criscenti
Stevenson	van de Krol	Crist	Bernhard	Mainardi
	Nelson	Woods	McNeill	Chellam

11:50 – 12:00 pm	Break
12:00 – 12:30 pm	Breakout session presentations and Group Discussion to identify Science Drivers and Mechanisms of Funding (Objective 1 Present, discuss and refine Science Drivers identified and their description)
12:30 – 1:30 pm	Lunch
1:30 – 1:45 pm	PNNL Overview
1:45 – 3:15 pm	EMSL Tour and Overview
3:15 – 3:30 pm	Overview of Breakout Session Charge: REFINEMENT OF GRAND CHALLENGES
3:30 – 5:00 pm	Break-out Session 4

Red 4	**Orange 4**	**Yellow 4**	**Green 4**	**Blue 4**
Roeselova	Lee	Noziere	Barney	Foster
Stahl	Francis	Chirik	Sanford	Weck
Geiger	Rosso	Blackwell	Criscenti	Martinez
Crist	van de Krol	Stevenson	Mainardi	Bernhard
Nelson	Woods		Chellam	McNeill

5:00 – 6:00 pm	Breakout session presentations and Group Discussion: Grand Challenges
6:00 – 6:15 pm	Wrap-up and Thank you! (Coates/Allen)
7:15 – 7:30 pm	Transportation to dinner - shuttle bus will leave from PNNL Guest House
7:30 – 11:00 pm	Dinner at Katya's Bistro & Wine Bar, 430 George Washington Way, Richland, WA (Phone: 509-946-7777)

Saturday, November 5, 2005

Check out by noon and depart for home