

PNL--10603

# **Pacific Northwest National Laboratory**

Operated by Battelle for the  
U.S. Department of Energy

**Pacific Northwest Laboratory**

**Director's Overview of Research  
Performed for DOE Office of Health  
And Environmental Research**

**June 1995**

**Prepared for the U.S. Department of Energy  
Under Contract DE-AC06-76RLO 1830**

**Pacific Northwest Laboratory  
Operated for the U.S. Department of Energy  
By Battelle Memorial Institute**



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**PACIFIC NORTHWEST LABORATORY**  
*operated by*  
**BATTELLE MEMORIAL INSTITUTE**  
*for the*  
**UNITED STATES DEPARTMENT OF ENERGY**  
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**MASTER**

Pacific Northwest Laboratory  
Richland, Washington 99352

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## List of Abbreviations

AAALAC	American Association for Accreditation of Laboratory Animal Care
ACP	Atmospheric Chemistry Program
AFM	atomic force microscope
ALE	Fitzner/Eberhardt Arid Lands Ecology
ANL	Argonne National Laboratory
ARM	Atmospheric Radiation Measurement
ARPA	Advanced Research Projects Administration
ASCOT	Atmospheric Studies in Complex Terrain
AWU	Associated Western Universities
AWU-NW	Associated Western Universities-Northwest
BEIR	Biological Effects of Ionizing Radiation (committee)
BES	Office of Basic Energy Sciences
BNL	Brookhaven National Laboratory
BPDE	benzo[a]pyrene diol epoxide
CART	Cloud and Radiative Testbed
CCARS	computer-controlled automated rain samplers
CEA	Commissariat a l'Energie Atomique
CEC	Commission of the European Communities
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CHAMMP	Computer Hardware, Advanced Mathematics, and Model Physics
CIRRC	Committee on Interagency Radiation Research and Policy Coordination
CRADA	Cooperative Research and Development Agreement
CSIRO	Commonwealth Scientific and Industrial Research Organization (Division of Atmospheric Research, Australia)
CZE	capillary zone electrophoresis
DNA	deoxyribonucleic acid
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
EDTA	ethylenediaminetetraacetic acid
EMSL	Environmental Molecular Sciences Laboratory
EPACT	National Energy Policy Act
EPR	electron paramagnetic resonance
EPRI	Electric Power Research Institute
ESD	Environmental Sciences Division
ESI-MS	electrospray ionization mass spectrometry

ESRC	Environmental Science Research Center
EULEP	European Late Effects Project
FTICR	Fourier transform ion cyclotron resonance
FY	fiscal year
FWP	field work proposal
GC	gas chromatography
GChM	Global Chemistry Model
GCM	general circulation model
GDB	Genome Data Base
GEC	Global Environmental Change
GIS	Geographic Information System
Gy	Gray
HMS	Hanford Meteorological Station
IAB	International Advisory Board
IAEA	International Atomic Energy Agency
IARC	International Agency for Research on Cancer
ICR	ion cyclotron resonance
ICR-MS	ion cyclotron resonance mass spectrometry
ICRP	International Commission on Radiological Protection
ICRU	International Commission on Radiological Units
IEA	International Energy Agency
IEEE	Institute of Electrical and Electronics Engineers
INEL	Idaho National Engineering Laboratory
IPCC	Intergovernmental Panel on Climate Change
IRB	Institutional Review Board
ITRI	Inhalation Toxicology Research Institute
kb	kilobases
keV	thousand electron volts
LANL	Los Alamos National Laboratory
LBL	Lawrence Berkeley Laboratory
LDRD	Laboratory Directed Research and Development
LET	linear-energy-transfer
LI	laser ionization
LLNL	Lawrence Livermore National Laboratory

MeV	million electron volts
MS	mass spectrometry
MSL	Marine Sciences Laboratory
NARE	North Atlantic Regional Experiment
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCI	National Cancer Institute
NCRP	National Council on Radiation Protection and Measurements
NEPA	National Environmental Policy Act
NFOM	near field optical microscope
NIH	National Institutes of Health
NIOSH	National Institute for Occupational Safety and Health
NIST	National Institute of Standards and Technology
NMR	nuclear magnetic resonance
NOAA	National Oceanic and Atmospheric Administration
NPBP	National Radiation Protection Board
NRA	National Radiobiology Archives
NRC	Nuclear Regulatory Commission
NREL	National Renewable Energy Laboratory
NSF	National Science Foundation
NTA	nitrilotriacetic acid
OECD	Organization for Economic Cooperation and Development
OGCM	ocean general circulation model
OHER	Office of Health and Environmental Research
OMIM	Online Mammalian Inheritance in Man
OPRR	Office for Protection from Research Risks
ORNL	Oak Ridge National Laboratory
OTD	Office of Technology Development
PLFA	phospholipid fatty acids
PNL	Pacific Northwest Laboratory
RAMS	Regional Atmospheric Modeling System
RBE	relative biological effectiveness
RCRA	Resource Conservation and Recovery Act
SAC	Scientific Advisory Committee
SCG	single-cell gel
SCR	stochastic-convective reaction
SERF	Subsurface Environmental Research Facility

SERS	Science and Engineering Research Semester
SFC	supercritical fluid chromatograph
SGM	Second-Generation Model
SRL	Savannah River Laboratory
SSP	Subsurface Science Program
TRAC	Teacher Research Associates
WNA	western North Atlantic

## 1.0 Program Summary

A significant portion of the research undertaken at Pacific Northwest Laboratory (PNL) is focused on the strategic programs of the U.S. Department of Energy's (DOE) Office of Health and Environmental Research (OHER). These programs, which include Environmental Processes (Subsurface Science, Ecosystem Function and Response, and Atmospheric Chemistry), Global Change (Climate Change, Environmental Vulnerability, and Integrated Assessments), Biotechnology (Human Genome and Structural Biology), and Health (Health Effects and Medical Applications), have been established by OHER to support DOE business areas in science and technology and environmental quality.

PNL uses a set of critical capabilities based on the Laboratory's research facilities and the scientific and technological expertise of its staff to help OHER achieve its programmatic research goals. Integration of these capabilities across the Laboratory enables PNL to assemble multidisciplinary research teams that are highly effective in addressing the complex scientific and technical issues associated with OHER-sponsored research. PNL's objectives are to

- bring our basic scientific and technological capabilities to bear on a wide range of applied science programs to enhance the effectiveness of these programs
- advance the frontiers of environmental molecular science research to provide the knowledge needed to strengthen PNL's research and development and application activities through the establishment of a state-of-the-art research user facility, the Environmental Molecular Sciences Laboratory (EMSL)
- understand the behavior of contaminants in subsurface, marine, and atmospheric environments
- improve understanding of environmentally important microbial systems
- enhance fundamental knowledge related to environmentally and industrially important processes, such as chemical separations and the behavior of complex fluids
- bring emerging supercomputing technologies to bear on modeling complex physical systems
- advance understanding of the health effects of chemical and radioactive substances
- establish and use alliances/collaborations with outside experts whose skills and capabilities complement our own strengths.

PNL research efforts increasingly are focused on complex environmental and health problems that require multidisciplinary teams to address the multitude of time and spatial scales found in health and environmental research. Using this multidisciplinary approach, PNL is able to directly support many

of the major programmatic objectives of OHER's Divisions of Environmental Sciences, Health and Life Sciences, and Medical Applications and Biophysical Research. PNL is currently engaged in research in the following areas for these OHER Divisions:

- Environmental Sciences
  - atmospheric radiation monitoring
  - climate modeling
  - carbon cycle
  - atmospheric chemistry
  - ecological research
  - subsurface sciences
  - bioremediation
  - environmental molecular sciences
- Health Effects and Life Sciences
  - cell/molecular biology
  - biotechnology
- Medical Applications and Biophysical Research
  - analytical technology
  - radiological and chemical physics.

Major PNL contributions to OHER strategic research programs are briefly described in the remainder of this section. These contributions and other OHER-sponsored research programs at PNL are described in detail in subsequent sections of the report.

**Environmental Processes.** PNL's environmental research is wide-ranging into the effects of natural events and human activities on the environment and on technologies to minimize environmental impacts and remediate damage caused by human activities. Our environmental research programs use state-of-the-art facilities to further our understanding of local- to global-scale effects on air quality and climate, and of subsurface and terrestrial systems; information critical to predicting the transport and transformation of toxic substances in the environment. PNL is also developing, with sponsorship from OHER, the EMSL as a major research center for collaborative research related to the environment.

Environmental research at PNL is focused on developing a fundamental understanding of key processes controlling chemical behavior and biological stress in terrestrial and subsurface systems. This understanding drives the development of emerging new concepts for subsurface remediation and for predicting landscape-level impacts from environmental restoration and global climate change. Unique intermediate-scale and field facilities, in conjunction with mathematical modeling and remote sensing, are used to examine the integrated effects of environmental processes, validate predictive models, and extrapolate results to the system level.



Examples of other Subsurface Science Program (SSP) research in progress include studies to 1) examine the mechanisms underlying interfacial reactions between mixed contaminants and mineral surfaces; 2) define the factors governing the presence and activity of microorganisms in the deep subsurface and their origins and movement over geologic time; 3) determine the processes underlying physical partitioning of vapors, solvents, and solutes in porous media; and 4) implement advanced experimental concepts for coupling and scaling fundamental molecular, cellular, chemical, and physical processes and their interactions to understand contaminant behavior in heterogeneous field environments.

Atmospheric research conducted at PNL is centered on two related areas, atmospheric chemistry and boundary layer meteorology. Major atmospheric chemistry studies focus on the fate of energy-related pollutants through research on atmospheric gas-phase and heterogeneous chemistry; cloud and aerosol chemistry, physics, and dynamics; and global-scale chemical transport modeling.

**Global Change.** PNL's Global Change Program directly supports the technical objectives of the Environmental Sciences Division on environmental change. Components of the Environmental Sciences Division represented at PNL include the Atmospheric Radiation Measurement (ARM) program; the Core Carbon Dioxide Research program; the Computer Hardware, Advanced Mathematics, and Model Physics (CHAMMP) program; the oceans research program; Global Change Integrated Assessment Research; and the quantitative links program. These programs have the common goal of improving our understanding of the physical, geological, chemical, biological, and social processes that influence the earth system so that national and international policymaking related to natural and human-induced changes in the earth system can be given a firm scientific basis. PNL continues to lead the planning and organization of the ARM program and the oceans research program, as well as assisting the Environmental Sciences Division with the implementation of CHAMMP. Each program involves a number of DOE laboratories and other agencies and strong participation from the university community.

PNL also plays a leading role in other long-term research thrusts that provide the scientific foundations on which the global change programs are based, from which energy-related air pollution assessments draw improved models, and with which safety evaluations at DOE sites reduce environmental uncertainties. This work comprises the Atmospheric Chemistry Program (ACP) and the Atmospheric Studies in Complex Terrain (ASCOT) program. The ASCOT program focuses on density-driven air circulations, turbulent mixing and dispersion in the atmospheric boundary layer, and microscale to mesoscale meteorological processes that affect air-surface exchange processes.

**Biotechnology.** A program has been initiated at PNL to model structure/function relationships in cytochrome P450 and haloalkane dehalogenase enzymes, with a goal of redesigning these enzymes for a variety of applications in bioremediation. Starting from a structure determined by x-ray crystallography, molecular dynamics simulations are being performed on the docking of both native and nonnative substrates in the enzyme active site. Predictions are then made on the effects of modifications in the enzyme active site on substrate specificity and catalytic efficiency, and site-directed mutagenesis procedures are being used to genetically engineer enzymes with modified active sites, followed by tests to determine the resultant changes in catalytic functionality.

Methods are being developed at PNL to aid in interpreting and understanding the vast amount of information being generated as a result of the human genome program. A graphics user interface called GnomeView has been developed to graphically represent 1) the hierarchy of available information from the chromosomal level, 2) the genetic and physical mapping level, and 3) the actual deoxyribonucleic acid (DNA) sequence level.

New approaches are also being developed at PNL with the potential for high-speed DNA sequencing based on mass spectrometry. In one approach, large single-stranded segments (1 to 20 kilobases) are transferred to the gas phase by an electrospray process that produces highly charged molecular ions. The ions are then trapped in an ion cyclotron resonance (ICR) cell in a high-magnetic field where a single molecular ion can be trapped, isolated, and nondestructively detected with high mass measurement accuracy.

**Health.** PNL health effects research ranges from the study of fundamental physical and chemical processes to the mechanisms by which hazardous physical and chemical agents affect living systems. Biological research in this programmatic area is addressed through a multilevel approach that incorporates studies from the molecular level to the whole-animal level. Emphasis is placed on understanding effects resulting from low-dose exposures that are characteristic of occupational and environmental situations. Integrated dosimetric, molecular, cellular, and experimental animal approaches are used to gain a quantitative understanding of fundamental mechanisms that underlie the effects of radiation and chemicals. PNL's program includes use of the unique single-particle microbeam irradiation system to determine the effects of individual radiation events in cells. The microbeam and other specialized exposure facilities are used in basic studies to test hypotheses concerning the interaction of chemical and physical agents with molecules in biological systems and the alteration of these molecules by the transfer of energy.

Our molecular and cellular research focuses on understanding the fundamental nature of damage by radiation and chemicals through studies of the molecular alterations produced in the DNA of cells exposed to these agents. A long-term objective of this research is the structural analysis of DNA damage induced by exposure of cells to radiation and chemicals. We apply new theoretical and spectroscopic approaches to understanding the mechanisms involved in mutagenesis, carcinogenesis, and developmental abnormalities through modeling three-dimensional structures of macromolecules and providing structural biology information that complements molecular biology research.

In radon research, in vitro studies incorporating radiation biophysics, dosimetry, and molecular and cellular biology to understand the mechanisms leading to radiation damage at the cell level are integrated with in vivo dose-effect studies, dosimetry and risk modeling, and carcinogenesis research. This effort is expected to provide insight into the elevated relative biological effectiveness of alpha particles, the dose-rate effects observed in high-linear-energy-transfer radiation, and the variations in relative biological effectiveness observed for different biological endpoints.

Life-span microdosimetric and pathobiologic studies of inhaled plutonium in rats and dogs, comparing metabolism and dose-effect relationship data for rats (life span approximately 3 years) with those for dogs (life span approximately 15 years), have provided insight into factors that must be considered in modeling and extrapolating animal data to humans. The results of these studies in rats and dogs exposed to inhaled plutonium and radon are being entered into the DOE National Radiobiology

Archives (NRA) at PNL to preserve individual animal dose-effects data and tissues from life-span animal studies for future analysis. The National Radiobiology Archives, developed and managed by PNL, consists of a computerized information system for dose-effects data, a repository for documents and other research records, and a tissue archive, integrated by a computerized inventory system.

PNL scientists are engaged in an OHER-sponsored research program that involves medical internal dosimetry and the search for new radioimmunoconjugates. The objectives of this program are to 1) provide internal dosimetry support to major medical facilities in their studies on the effectiveness of radiolabeled antibodies in the diagnosis and treatment of cancer; 2) develop improved methods for estimating radiation doses to tumors and normal tissues from incorporated radiolabeled antibodies, hormones, and growth factors; and 3) develop new alpha-particle-emitting immunoconjugates for use in therapy. PNL is currently conducting dosimetric assessments in support of the lymphoma and leukemia clinical trials at the Fred Hutchinson Cancer Research Center and the University of Washington in Seattle, and other clinical studies at the Virginia Mason Cancer Clinic (Seattle) and the National Institutes of Health (Bethesda, Maryland). We are undertaking new research in radiochemistry and macrocyclic ligand chemistry, immunology, and production of novel alpha emitters to develop more effective alpha-emitting radioimmunoconjugates for cancer treatment. We are also studying new laser-based thermoluminescent dosimetry systems and associated instrumentation for direct measurements of dose and dose rates in the body from medically administered, high-dose levels of radiolabeled antibodies.

## **2.0 Program Organization, Facilities, and Resources**

### **2.1 Organization and Management of OHER Programs**

The OHER-sponsored research at PNL is managed through a central program office that interacts with scientists conducting the research within a research line organization. The line management functions (including conduct of operations and Environmental Safety and Health) are provided by six major laboratory research organizations each led by an Associate Laboratory Director. Programmatic management of the OHER research is provided by the Office of Energy Research (OER) Program Office, managed by B. R. Stults. The OER Program Office reports to M. L. Knotek, Associate Laboratory Director for Environmental and Energy Research. The relationship between the PNL line management and the Program Office is shown in Figure 2.1 and Figure 2.2 which lists the OHER subprogram managers who are responsible for providing primary client point of contact to the various headquarters program offices in OHER.

The recent changes in the organization of PNL and the formation of a single program office for all of Energy Research were instituted to provide a more streamlined organization focused on DOE's missions in science and technology, environment, energy, and national security. The OER Program Office is expected to provide the following benefits to the OHER Program Divisions and the research staff at PNL.

1. High-level guidance and focus to PNL's basic science programs, which will lead to early identification of future research opportunities and synergistic contributions of current research to problems requiring multidisciplinary solutions.
2. A single point of contact at PNL to oversee, coordinate, and integrate our interactions with the various OHER program offices.
3. Effective dissemination of knowledge gained from OHER-sponsored research throughout PNL and integration of this new knowledge into all of the Laboratory's research.
4. A decrease in PNL's business costs by eliminating duplication, reducing requirements, and streamlining responsiveness to the customer.
5. An increase in PNL's visibility to the client, academia, local and regional communities, and other national laboratories.

## Pacific Northwest Laboratory

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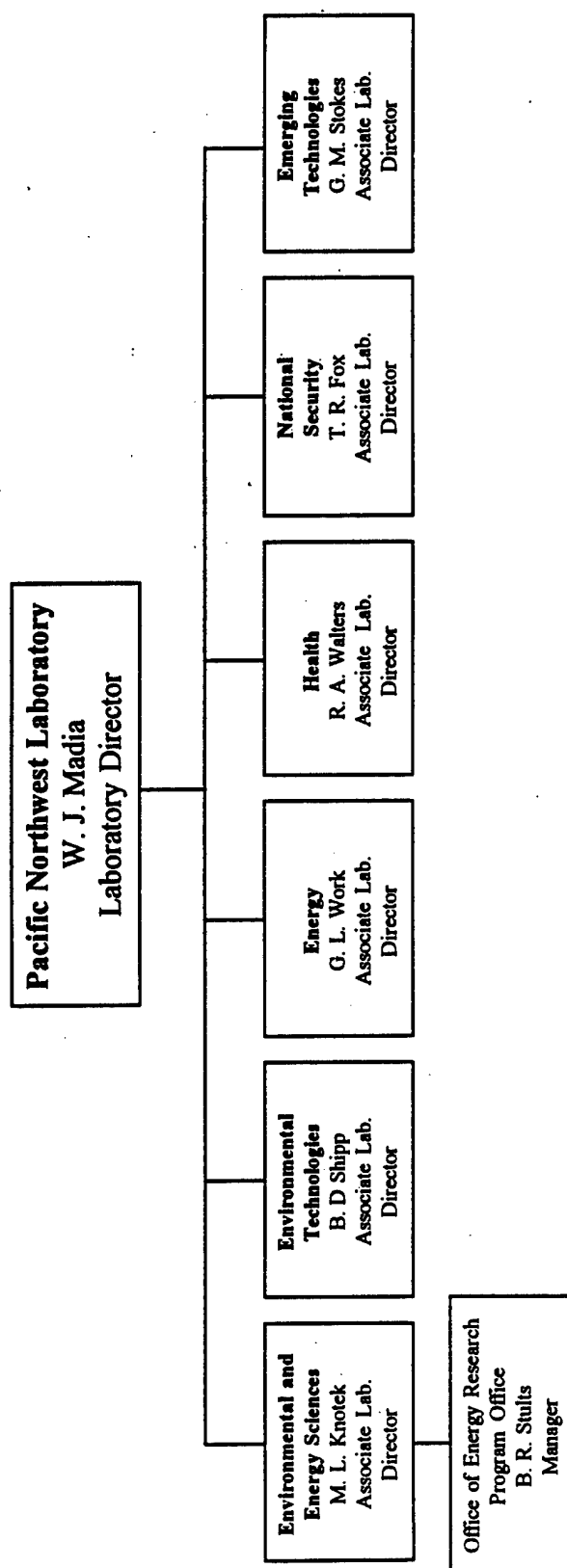


Figure 2.1. PNL Line Management and Relationship to Program Office

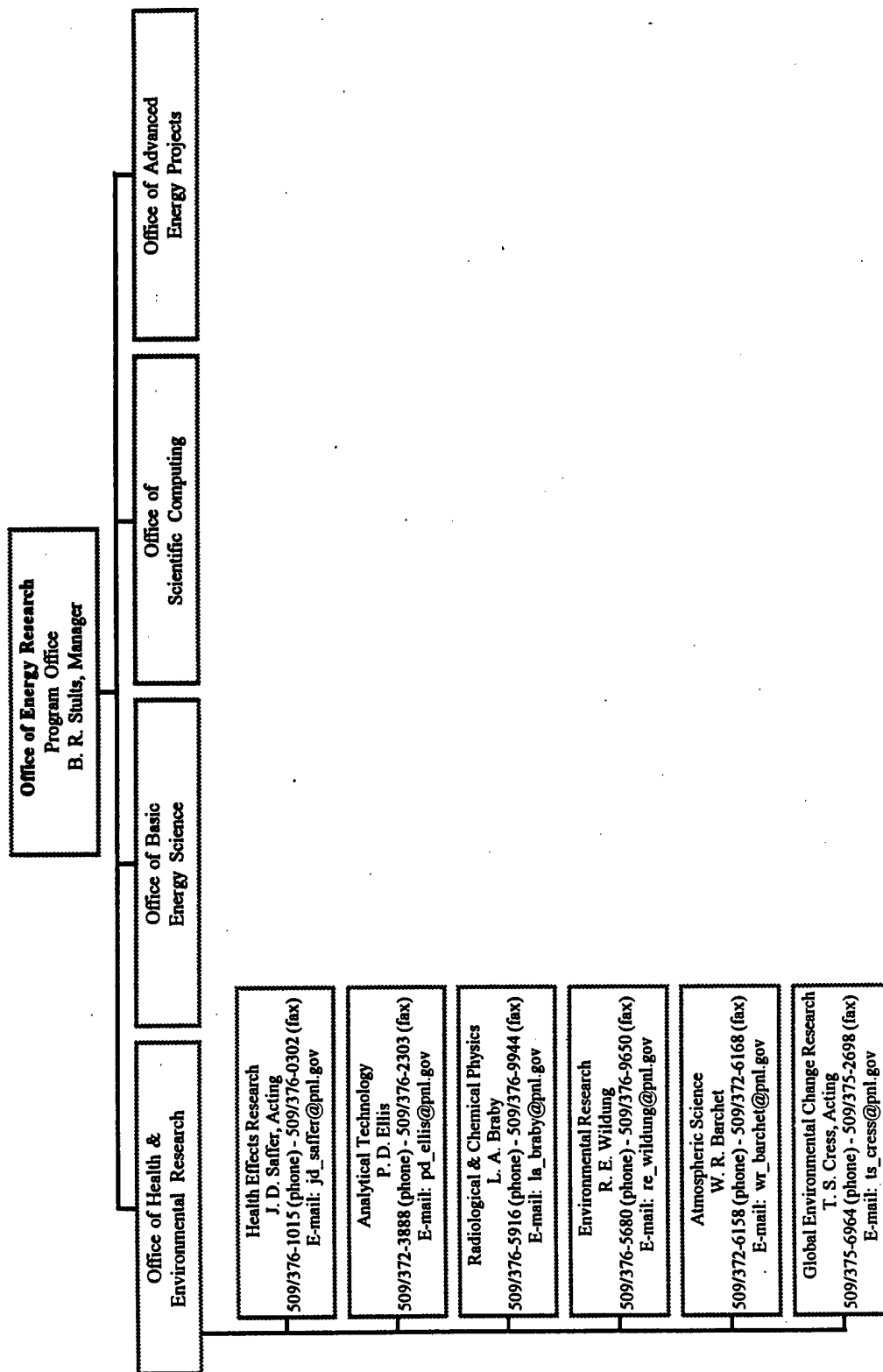


Figure 2.2. Subprogram Managers Providing Primary Client Point of Contact

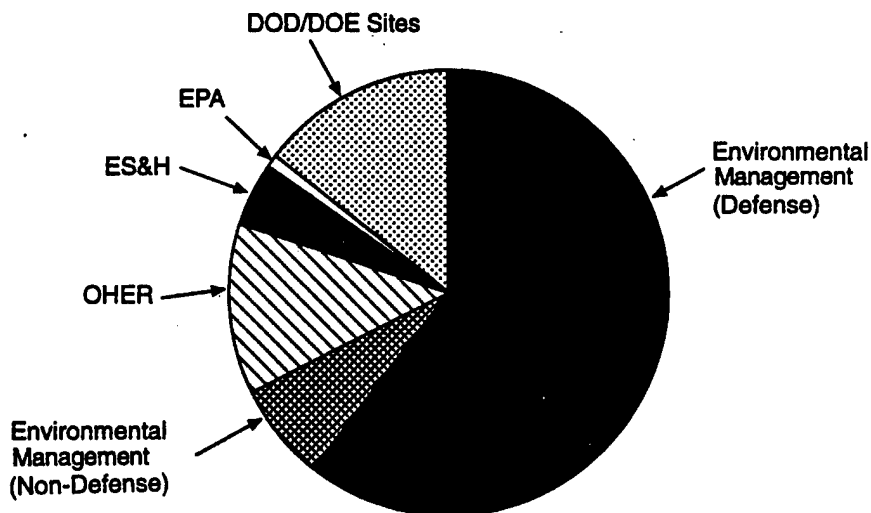
## 2.2 Budget Information

**Table 2.1.** Budget Data for FY 1993, 1994, and 1995<sup>(a)</sup>

Budget Authority Data <sup>(b)</sup>		FY 1993	FY 1994	FY 1995
KP-01	Analytical Technology	725	690	333
KP-02	Environmental Research	8,908	9,617	9,460
KP-03	Health Effects	4,530	3,655	3,975
KP-04	General Life Sciences	862	1,135	1,331
KP-05	Global Change Research	17,660	22,442	19,043
KP-06	Medical Applications	0	0	229
Total		32,685	37,539	34,371

(a) \$K

(b) Reduction in budget authority for FY 1995 was largely offset by carry-over of \$8,385K. (Carry-over going into FY 1994 was only \$5,353.)



**Figure 2.3.** Sponsors of Current Programs

## 2.3 Personnel

The numbers of staff in various categories working on OHER-sponsored projects are listed in Table 2.2. OHER research programs have access to the full capabilities of the laboratory.

**Table 2.2. Staff Working on OHER-Sponsored Projects<sup>(a)</sup>**

	<b>FY 1993</b>	<b>FY 1994</b>	<b>FY 1995</b>
Principal Investigators	54	58	58
Scientists <sup>(b)</sup>	124	132	133
Technicians <sup>(c)</sup>	13	12	12
Other <sup>(d)</sup>	46	46	46

(a) In FY 1993, \$9.7M (~30%) and in FY 1994 and 1995, \$10M (~35%) of PNL's OHER budget, primarily in the ARM Program, is for subcontracts with other organizations. The numbers in this table do not include staff working on those subcontracts.

(b) Includes principal investigators, other scientific staff, and postdoctoral fellows.

(c) Includes animal care staff.

(d) Includes administrators, secretaries, clerks, and financial staff.

## 2.4 Facilities and Resources

Biological and environmental studies are conducted primarily in two major laboratory buildings: one is a DOE facility (120,000 ft<sup>2</sup>), and the other is a Battelle facility (100,000 ft<sup>2</sup>). Additional studies are conducted in the 45,000-ft<sup>2</sup> Battelle Marine Sciences Laboratory (MSL), which is the only marine laboratory in the national laboratory system. Other biological, environmental, and physical sciences research is conducted in various facilities on the Hanford Site. PNL is unique among the OHER laboratories in that research is performed in Battelle-owned or leased private facilities in addition to DOE-owned facilities. A brief description of the total facilities used for OHER research is given in Table 2.3. Most of these facilities are available on a program-collaborative basis for use by nonstaff research personnel who qualify for access to the Hanford Site.

Facilities devoted specifically to environmental research include the geochemistry, microbiology, hydrology, plant physiology, and computational laboratories, a wind-tunnel facility of advanced design for the study of surface interactions of aerosols and gases, the intermediate-scale Subsurface Environmental Research Facility (SERF), and the Fitzner/Eberhardt Arid Lands Ecology (ALE) facility, all in the Richland area, and the MSL at Sequim, Washington. The environmental laboratories are uniquely equipped for studies in subsurface, terrestrial, freshwater, or marine environments at the chemical, cellular, or whole-organism level. Staff at the MSL have laboratory and computational facilities for conducting research into chemical, biological, and physical oceanography. A new laser confocal microscope is providing the basis for studies of microbial colonization and function in three dimensions and as a function of time. In the wind-tunnel facility, laser optical methods provide nonintrusive



characterization and control of gas composition ( $O_2$ ,  $CO_2$ ,  $CO$ ,  $SO_2$ ,  $NO_x$ ,  $O_3$ , and other gases). Facilities and equipment are also available for examination of gas exchange and aerosol interception, as well as definition of effects on plants and animals.

The 127-mi<sup>2</sup> ALE Reserve, fenced and under surveillance, provides an outdoor laboratory for extrapolation and validation of concepts and laboratory data in the natural environment. Also, the 575-mi<sup>2</sup> Hanford Reservation has increasingly served as an outdoor laboratory for studies of the effects of waste disposal on subsurface and terrestrial environments, including unique deep exploration for useful microorganisms and the effects of surface disturbance on ecological communities.

Studies of the potential health consequences of exposure to radiation and chemical toxicants related to energy production are conducted in large and small animals, in microorganisms, in cultured mammalian cells, and in DNA and other molecular structures. Animal exposure modes include inhalation, ingestion, injection, and dermal application. Facilities are available for exposure of large and small animals via inhalation of radionuclides or chemicals. Special exposure systems are used for exposure of animals and cells to radon, radon progeny, and cigarette smoke. These exposure systems also are being used by researchers from other DOE-supported institutions for radon-progeny exposures. Special accelerator-based irradiation facilities are also available for studies involving high-linear-energy-transfer (LET) and high-dose-rate, low-LET exposures. These facilities provide charged particles ( $H^+$ ,  $He^{2+}$ ,  $C^+$  . . . ) with energies from a few thousand electron volts (keV) to several million electron volts (MeV), as well as monoenergetic neutrons and high-dose-rate x-ray and electron-exposure capabilities. Special features include a wide variation in dose rates (a few microgray [ $\mu$ Gy] per second to 100 megagray [MGy] per second), plus capability for split-dose measurement with 1-nsec resolution, and a range in radiation quality from low-LET x rays and fast electrons (2 MeV) to neutrons and high-LET heavy charged particles. Facilities are also available for exposure of cell cultures and animals to magnetic fields and electric fields under carefully controlled conditions. Equipment and facilities for radionuclide counting, high-resolution mass spectrometry (MS), gas chromatography (GC), supercritical fluid chromatography (SFC), electron paramagnetic resonance (EPR) spectroscopy, capillary zone electrophoresis (CZE), and laser ionization (LI) combined with MS are used to determine toxicant doses to whole animals, animal tissues, single cells, and macromolecules. In addition, ultraviolet, infrared, Fourier-transform infrared, and nuclear magnetic resonance (NMR) spectrometers are available for use to characterize biological materials in native and perturbed states. Analytical techniques such as video image analysis, flow cytometry and cell sorting, and transmission and scanning electron microscopy provide sensitive analysis of biological response. PNL has laboratories and instruments for molecular biology research including ultracentrifuges, liquid chromatographs, gel electrophoresis, and DNA extractors, synthesizers, and sequencers.

Construction of the EMSL began in July 1994. On completion in 1997, this major facility will bring a suite of capabilities beyond those offered by current state-of-the-art instruments. The facilities and research conducted in this 200,000-ft<sup>2</sup> facility will be focused on environmental applications. Some of the equipment to be housed in the EMSL has been purchased and is under further development. This equipment is available for programmatic research on a limited basis. A more complete description of the EMSL is found in Section 5 of this report.

A renovated space in the Life Sciences Laboratory I (3500 ft<sup>2</sup>) provides an NMR and pulsed EPR spectroscopy facility, which greatly expands capabilities for structural and dynamic macromolecular investigations. Five NMRs, which include a state-of-the-art, 750-MHz narrow-bore instrument, along with a 500-MHz narrow-bore instrument, provide new capabilities for studying the structure of DNA and proteins in solution. Solid-state protein structure determination is provided by the 500-MHz, 400-MHz, and 300-MHz wide-bore instruments, which also permit frequency-dependent studies. A new pulsed EPR spectrometer will enable the characterization of paramagnetic molecules and free radicals not amenable to NMR techniques.

Major equipment for atmospheric sciences research and support includes the Hanford Meteorology Station (HMS), a mesoscale network of meteorological sensors linked to HMS by radiotelemetry, and a field sampling grid for dispersion and deposition experiments; turbulence and boundary-layer remote sensing and profiling instrumentation; a mobile network of computer-controlled automated rain samplers (CCARS); an instrumented Grumman Gulfstream-1 turboprop research aircraft for measuring variables in meteorology, cloud physics, trace gases, and cloud chemistry; and a cluster of IBM RISC System 6000 computers and a network of Sun workstations (providing access to other local and distributed computing resources) for accumulating atmospheric databases and modeling atmospheric processes.

**Table 2.3. Major Facilities at Pacific Northwest Laboratory Related to the Office of Health and Environmental Research Program**

Facility	Size <sup>(a)</sup> (ft <sup>2</sup> )	Occupants	Major Features
<b>DOE-Owned Facilities</b>			
<b>100 Area</b>			
WBF-1, WBF-11	2,000	0 <sup>(b)</sup>	Boat and storage facilities
<b>200 Area</b>			
242-B Bldg	2,700	0 <sup>(b)</sup>	Particle research; burn chamber
<b>300 Area</b>			
326	50,000	2	Capillary zone electrophoresis-mass spectrometers; ultrasensitive orthogonal time-of-flight mass spectrometer; ion trap mass spectrometer; triple quadrupole mass spectrometer; high mass range mass spectrometer
329 Bldg	37,000	50	Physical sciences; low-level radiochemical analysis and counting labs; neutron multiplier facility; mass spectrometer and supercritical fluid chromatography laboratory; capillary zone electrophoresis laboratory

Table 2.3. (contd)

Facility	Size <sup>(a)</sup> (ft <sup>2</sup> )	Occupants	Major Features
Life Sciences Laboratory I (331 Bldg)	120,000	130	Nuclear magnetic resonance spectrometry laboratory; molecular biology laboratories; cell culture facilities; cell biology laboratories; radiochemistry laboratories; subsurface environmental research facility; applied microbiology laboratory; confocal microscopy facilities; gamma-ray exposure facility; aquatic wet laboratories and fish breeding facilities; animal care facilities; electron microscope facility; flow cytometry laboratory; Life Sciences branch library
331-A Bldg	2,800	0	To be demolished
331-B Bldg	4,200	0 <sup>(b)</sup>	Animal care facility
331-C Bldg	3,000	0 <sup>(b)</sup>	Equipment and supply storage
331-D Bldg	1,300	0 <sup>(b)</sup>	Radon calibration facility (planned)
331-E Bldg	1,500	0 <sup>(b)</sup>	Greenhouse
331-F Bldg	1,100	0 <sup>(b)</sup>	Equipment and supply storage
331-G Bldg	1,200	0 <sup>(b)</sup>	Interim facility for OHER National Radiobiology Archives
331-H Bldg	3,000	1	Closed-loop wind tunnel and aerosol measurement equipment for exposures of plants and soils to toxic materials including plutonium; laser optical sizing in real time
331-J Bldg	384	0 <sup>(b)</sup>	Waste incineration facility
3720 Bldg	29,000	24	Material sciences; five radiochemistry labs; wind tunnel for particle deposition
3745-A Bldg	1,277	0 <sup>(b)</sup>	Pulsed 2-MeV electron accelerator
3745-B Bldg	6,500	2	Positive ion accelerator with switching capability to multiple target areas; mono-energetic neutron irradiation facilities; charged-particle microbeam (5- $\mu$ m resolution)
3746, 3746-A Bldgs	5,000	13	Radiological physics; six cellular and molecular biology labs; offices
3767 Bldg	2,839	11	Computer and graphics laboratory for epidemiology and biometry staff
600 Area			
622 Bldg	3,000	0 <sup>(b)</sup>	410-ft meteorological tower with tracer release platforms and air-sampling grid for diffusion deposition modeling; 10 small support facilities
622-F Bldg	3,000	0 <sup>(b)</sup>	Radar profiler with radio acoustic sounding system IBM RISC 6000 computer for data processing and emergency models

Table 2.3. (contd)

Facility	Size <sup>(a)</sup> (ft <sup>2</sup> )	Occupants	Major Features
622-R	9,000	6	Atmospheric sciences; meteorological records; weather forecasting; two analytical labs; sodar
Telemetry Network	Dispersed over ~560 mi <sup>2</sup>	0 <sup>(b)</sup>	Meteorological measurements network for wind field and temperature input to emergency response system; includes three 200-ft meteorological towers, four Doppler acoustic sounders, 244 meteorological masts
Fitzner/Eberhardt Arid Lands Ecology Reserve	127 mi <sup>2</sup>		Unique, protected ecological reserve for examining the structure and function of shrub-steppe ecosystems over a broad range in altitude meteorology, soil types, and plant and animal communities
Mobile Ecology Laboratory	240	0 <sup>(b)</sup>	Plant ecophysiology research (gas exchange)
646 Bldg	800	0 <sup>(b)</sup>	Lab for aquatic and terrestrial research
6652-E	800	0 <sup>(b)</sup>	Garden shed (garage)
6652-G Bldg	6,800	0 <sup>(b)</sup>	Archived samples
6652-H Bldg	3,800	6	Six radiochemistry labs; growth chambers; gamma-radiation facilities
6652-I Bldg	4,200	7	Nonradiochemical lab
6652-J Bldg	7,800	3	Plant growth chambers and analytical labs; sample storage
6652-M Bldg	700	0 <sup>(b)</sup>	Two labs for processing and storing animal tissue samples to be examined for low-level radioactive material
6652-C Bldg	6,500	2	Space sciences labs (dark rooms, computer lab, offices); storage; support for optical telescope
Rattlesnake Mountain Observatory	800	0 <sup>(b)</sup>	31-in. optical telescope
Gulfstream-1 aircraft	-	0 <sup>(b)</sup>	Twin-turboprop aircraft outfitted with real-time and integrating sensors for atmospheric turbulence, chemistry, aerosol, and cloud research
3000 Area			
Life Sciences Laboratory II	100,000	120	Animal care facility with clean/regulated corridor system; HEPA filtration; surgical suite, autopsy area; soil microbiology, plant physiology, and subsurface organic chemistry laboratories; computer-based animal inhalation exposure suites; organic chemistry laboratory; biometrics VAX 11/780; offices

Table 2.3. (contd)

Facility	Size <sup>(a)</sup> (ft <sup>2</sup> )	Occupants	Major Features
PSL	1,800	3	High-field (7-tesla) high-resolution ion cyclotron resonance mass spectrometer
RRC Annex <sup>(c)</sup>	9,300	10	Animal care facility; electric- and magnetic-field exposure systems; electronics, behavioral physiology labs
RTL-520	56,000	76	80 offices; 14 laboratories, most with radio-chemical capabilities; soil chemistry laboratories
Research Operations Bldg	77,000	9	228 offices
Sequim, Washington			
Marine Sciences Laboratory	45,000	35	Wet lab; analytical lab complex; 20 radio-analytical labs; diagnostic center (marine diseases)
<b>Leased Private Facilities</b>			
<b>3000 Area</b>			
ISB 1 & 2	110,000	8	ARM Experiment Center; 8 offices
2400 Stevens Bldg	73,000	2	Four labs; 2 offices
Sigma Bldgs	46,000	137	40 OHER offices; 8 chemistry analytical labs; computer facilities
<b>Pasco Airport</b>			
Airplane hangar	8,000	0 <sup>(b)</sup>	Shelter and maintenance facilities for Grumman Gulfstream-1 turboprop research aircraft
Office, shop, and storage area	2,000	0 <sup>(b)</sup>	

(a) Total square footage of facility, includes both OHER and non-OHER space.

(b) No permanent occupants.

(c) No current OHER projects in this facility.

## **3.0 Research Management Practices**

### **3.1 Advisory Committees and Program Reviews**

At PNL, internal and external reviews are conducted to set program directions, establish priorities, and ensure scientific quality. PNL has several standing advisory panels (see Table 3.1), e.g., the EMSL Advisory Panel, that meet at regular intervals. These panels perform a variety of functions varying from conducting peer technical review (including bringing in outside expert consultants) to providing advice relative to future program direction. PNL also assembles, at DOE-Headquarters request, peer review panels to provide in-depth review of specific projects and programs (e.g., EMSL project reviews) and participates in peer review panels established by DOE-Headquarters (e.g., Subsurface Science Program). A list of project reviews is provided in Table 3.2.

Individual programs within OHER are regularly reviewed externally to assess program design and objectives, and larger, focused programs are subject to regular oversight. Programs for which oversight is conducted include

1. ARM—Annual review of program content, objectives, and performance by the JASONs of ARPA (Advanced Research Projects Administration). Results of the reviews are published in a formal letter report to the DOE program manager, who is responsible for responding accordingly.
2. CHAMMP—External peer review of program content, objectives, and performance on at least a biennial basis. Reviews have been conducted by the JASONs and by selected ad hoc groups. Formal reports on the review process are written and responded to by the DOE program manager.

In addition to DOE oversight, PNL's Global Studies Program has established an International Advisory Board (IAB) of very senior scientists and environmental policy experts to review and assess PNL's integrated global environmental change program. The IAB meets on a regular basis and advises senior PNL management on the strategy and content of the program. The IAB members and their affiliations are listed in Table 3.1.

### **3.2 Performance Measures**

There are five systems used at PNL to review the research quality, productivity, and mission relevance of the programs sponsored by the OHER.

First, PNL takes a prospective view of major research programs using both external and internal advisory panels to evaluate PNL's research portfolios and develop recommendations for future program direction and development. A high level PNL Advisory Committee (see Table 3.1 for members' names) meets three times a year to review the Laboratory's overall strategic intent and provide

**Table 3.1. PNL Advisory Committee Membership****I. Standing PNL Advisory Panels**

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**A) PNL Laboratory Advisory Committee**

Governor Richard Celeste  
Chairman  
Celeste & Sabety

Dr. Richard Balzhiser  
President & CEO  
Electric Power Research Institute (EPRI)

Mr. Erich Bloch  
Distinguished Fellow  
Council on Competitiveness

Mr. Kenneth Davis  
Former Deputy Secretary of  
Energy

Mr. Jess DiAx  
Manager, Strategic Marketing  
Motorola Inc.

Honorable Daniel Evans  
Chairman  
Daniel J. Evans Associates

Dr. Steve Gage  
President  
Cleveland Advanced Mfg Program

Dr. Fredrick Humphries  
President  
Florida A&M University

Ms. Pamela Linton  
President & CEO  
Pollution Solutions

Mr. Gene McBrayer  
Former CEO  
Exxon Chemicals

Dr. Dwight Sangrey  
Immediate Past President  
Oregon Graduate Institute

Dr. Samuel Smith  
President  
Washington State University

Dr. Elizabeth Zinser  
President  
University of Idaho

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Table 3.1. (contd)

## B) EMSL Advisory Panel

Dr. David A. Dixon  
Central R&D Department  
Experimental Station  
E.I. DuPont de Nemours

Dr. Jerry Ebner\*\*  
Monsanto Company

Professor Robert Griffin  
Department of Chemistry  
Massachusetts Institute of Technology

Dr. James B. Harsh  
Assoc. Prof. of Crops & Soils  
Washington State University

Professor Steve Kevan  
Department of Physics  
University of Oregon

\* Advisory Panel Chair 1990-1994

\*\* Advisory Panel Chair 1995-present

Dr. Mel Koch  
Analytical Sciences Lab  
Dow Chemical USA

Professor Edward Lazowska  
Department of Computer Science  
and Engineering  
University of Washington

Professor John Simon  
Department of Chemistry  
University of California

Dr. Peter R. Taylor  
San Diego Supercomputer Center

Dr. Robert O. Watts\*  
Department of Chemistry  
University of Washington

## C) EMSL - Molecular Science Computing Facility Advisory Committee

Professor Edward F. Hayes  
The Ohio State University

Professor Rick Dahlquist  
University of Oregon, Eugene

Dr. David A. Dixon  
Central R&D Department  
Experimental Station  
E.I. DuPont de Nemours

Professor William Jorgensen  
Yale University, New Haven

Professor Edward Lazowska  
Department of Computer Science and Engineering  
University of Washington

Dr. C. William McCurdy  
NERSC  
Lawrence Livermore National Laboratory

Dr. Mark S. Gordon  
Department of Chemistry  
Iowa State University

Professor Ken Merz  
Pennsylvania State University  
University Park

Professor John Moulton  
University of Maryland Biotechnology Institute  
Rockville



**Table 3.1. (contd)****D) Global Studies International Advisory Board**

Professor Harvey Brooks  
 Professor of Technology & Public Policy  
 John F. Kennedy School of Government  
 Harvard University

Hon. Robert McNamara  
 USA

Ambassador Richard Benedick  
 World Wildlife Fund  
 USA

Professor the Lord Desai of St. Clement Danes  
 The Centre for the Study of Global Governance  
 London School of Economics

Professor George Golitsyn  
 Institute of Atmospheric Physics  
 Russian Academy of Sciences

Professor Richard S. Odingo  
 Co-Vice Chair, IPCC/WG III  
 Department of Geography  
 University of Nairobi

Dr. Dipak Gyawali  
 Pragma (Member) of RONA

Lord Sherfield  
 House of Lords  
 United Kingdom

Dr. Jiro Kondo  
 RITE

Professor Thomas Schelling  
 School of Public Affairs  
 University of Maryland at College Park

Dr. Hoesung Lee  
 Korea Energy Economics Institute

Peir Vellinga, Ph.D.  
 Director, Instituut voor  
 Milieuvraagstukken  
 The Netherlands

Dr. Tom Malone  
 Sigma Xi  
 USA

Ernst U. von Weissacker, Ph.D.  
 President  
 Wuppertal-Institut  
 Germany

Table 3.1. (contd)

## II. Project Review Committee Membership

## A) EMSL Project Review - February 2-3, 1994

Scientific and Technical Consultants	DOE Members	
William Bleam, University of Wisconsin	Dan Lehman, ER-65	John Neath, RL
Dennis Hall, LBL	Robert Marianelli, ER-14	Mike Riches, ER-74
Larry Jackson, MACTEC	Steve Barnhart, ER-14	Eddie Sims, ER-65
Mel Koch, Dow Chemical	Harry Bell, RL	Ted Tomczak, ER-14
William McCurdy, LLNL	Sondra Kevelier, FM	Ron Yourd, ER-65
Edward Temple, ANL	Tom Kitchens, ER-30	Robert Zich, ER-64
Robert Watts, University of Washington		
Mary Wheeler, Rice University		
Michael White, University of Texas		

## B) EMSL Project Review - November 2-4, 1994

M. Teresinski, ER-13	H. Bell, DOE-RL
R. Marianelli, ER-14	Dr. Beverly Hartline, CEBAF
S. Barnhart, ER-14	Dr. Ed Temple, ANL
T. Kitchens, ER-30	Dr. William McCurdy, NERSC
M. Osinski, ER-63	Dr. Ron Gould, SSRL
R. Zich, ER-64	Dr. George Fisk, SNL
D. Lehman, ER-65	Dr. David Rakestraw, SNL
J. Carney, ER-65	Professor John Simon, University of California
R. Eicher, ER-73	Dr. William H. Woodruff, LANL
M. Riches, ER-74	Dr. Gordon E. Brown, Jr., Stanford University
M. Briodo, ER-74	Dr. Howard Padmore, LBL
B. Parra, ER-74	Dr. Leonard C. Feldman, AT&T Bell Labs
E. Sims, FM-50	Professor Robert O. Watts, University of Washington
V. Bohanan, FM-50	Dr. Paul E. Bayer, Energetics Inc.
B. Wunderlich, CH-APS	Ray Stults, RL-PNL
J. Neath, DOE-RL	Thom Dunning, RL-PNL
J. Axtell, DOE-RL	

## C) Structural Biology Review Panel - April 18, 1995

This review was organized by D. A. Smith and M. Broido of OHER.

R. Dahlquist University of Oregon, Eugene	J. Moul University of Maryland Biotechnology Institute Rockville
W. Jorgensen Yale University, New Haven	W. Trager University of Washington Seattle
K. Merz Pennsylvania State University University Park	

**Table 3.2. PNL Review Committees and Program Reviews**

Committee	Meeting Date	Report Issued
MSCF Advisory Committee	July 15-16, 1994	Meeting minutes available
MSCF Advisory Committee	March 21-22, 1995	Meeting minutes available
EMSL Advisory Committee	September 22, 1994	Meeting minutes available
EMSL Advisory Committee	March 23-24, 1995	Meeting minutes available
EMSL Project Review	February 2-3, 1994	Report issued
EMSL Project Review	November 2-4, 1994	Report issued
Environmental Science Research Center Review, Lewes, Delaware	April 7-8, 1994	Report issued
Subsurface Science Program		
DOE SSP Heterogeneity Subprogram Review, Norfolk, Virginia	October 11-13, 1993	Report issued
DOE SSP Special Projects Review, Annapolis, Maryland	January 17-18, 1995	Report issued
DOE SSP Multiphase Fluid Flow Subprogram Review, Gaithersburg, Maryland	January 24-25, 1994	Report issued
DOE SSP Colloids Subprogram Review, Gaithersburg, Maryland	February 14-15, 1994	Report issued
Bacterial Transport Subprogram	February 16-17, 1994	Report issued
Deep Microbiology-Microbial Ecology Subprogram	April 18-20, 1994	Report issued
Co-Contaminant Chemistry Subprogram	June 7-8, 1994	Report issued
Structural Biology Program	April 18, 1995	Report pending

forward-looking advice relative to the balance of PNL's support for national goals, to assess trends in scientific, technical, economic, environmental, social, and political affairs; and to assist in the identification of and response to trends and developments which bear on strategic planning for future opportunities and challenges. The Laboratory assembles internal review panels to review existing OHER programs and develop recommendations for future program development and redirection. For example, in 1994, an internal review of PNL's health effects research programs resulted in the initiation of a major shift in program direction to more directly couple the health effects research with the emerging new capabilities in the EMSL. The recommendations of this review group were instrumental in securing Laboratory Directed Research and Development (LDRD) funds to initiate new research

topics and to form new research collaborations. The scope of PNL's new research directions were presented to Dr. David Smith in April 1995 and a research proposal is being prepared for submittal and peer review by the Health Effects and Life Sciences Division.

Second, the Laboratory annually submits to the Office of Energy Research a 5-year Institutional Plan. A draft plan is reviewed by both DOE-RL and DOE-HQ and it forms the basis for the annual site visit by the head of the Office of Energy Research and representatives from major OER Program Offices, including OHER. The on-site visit followed by review and acceptance of PNL's Institutional Plan serves as approval for the Laboratory's strategic intent and the direction of the Laboratory's research programs. PNL, in conjunction with the Richland Operations Office, develops an Annual Appraisal Plan. Performance against several metrics with input from the DOE-HQ Program Offices provides the basis for the Laboratory's annual performance rating. Below is a summary of the performance measures which directly relate to OHER's programs at PNL.

- **FY 1995 PNL Appraisal Plan Expected Results.** PNL, in collaboration with industrial and university partners, will conduct nationally significant research in fundamental science and in technology development and application that provides the basis for innovative and effective technical solutions for DOE and national needs. In particular, PNL will
  - develop significant new knowledge in, and maintain relevant leading-edge fundamental science capabilities for the molecular, materials, environmental, biological, and computer sciences
  - ensure the technical quality and continued relevancy of our core competencies of Integrated Environmental Research, Process Science and Engineering, and Energy Systems Development
  - enhance current and develop new core technical capabilities as appropriate that closely support the present and future DOE and national science and technology needs
  - help provide a technically trained and diverse work force for the nation and enhance American scientific and technical literacy.

PNL and its partners will develop and deploy impactful solutions for major environmental problems. In particular, PNL will

- provide a defensible basis for setting environmental management priorities and targets, and establish technically, financially, and managerially sound approaches to meeting those targets
- develop comprehensive solutions which are faster, lower cost, or more effective while preventing future problems
- achieve excellent programmatic, schedule, and budget performance on environmental management programs.

PNL will deliver the EMSL as a preeminent collaborative research facility, with operation to begin in the fall of 1997. In particular, PNL will ensure that

- construction of the conventional facility will be completed on schedule within the agreed upon construction cost
- the EMSL will provide the maximum possible scientific capabilities within recognized technology limits and the total project cost
- the EMSL will possess a full complement of research programs and staff of the highest scientific quality by the beginning of FY 2001
- scientific research conducted in the EMSL will have a demonstrable impact on DOE's missions, especially its environmental quality mission, within three years of initiation of operation
- the EMSL will be fully subscribed by outside users by the beginning of FY 2001.

PNL will manage its facilities and conduct work in a manner that protects the health and safety of our staff and the public and the environment. In particular, PNL will establish an effective, efficient, integrated, and graded approach to Environmental Safety and Health and Conduct of Operations requirements that is a competitive advantage for PNL.

• **Performance Indicators.**

- inventory of significant accomplishments in the Science and Technology mission, including advances in fundamental knowledge, creation of significant technology, and development of premier technical capabilities and facilities
- results of peer reviews conducted during 1995 of major science and technology programs
- results of the EMSL advisory panel evaluation of PNL progress in acquiring and developing staff and research capabilities in line with program requirements and facility design specifications and PNL progress in developing the EMSL user community
- level of collaboration with educational organizations, including number of joint research partnerships with universities, number of educational appointees at PNL, and the number of partnerships with educational entities as part of the state of Washington's systemic reform process, as part of the School-to-Work program, or the Goals 2000 program
- technical community recognition of PNL staff, including scientific awards, professional society recognition, and technology awards.

Third, each year PNL submits dozens of requests to OHER for program/project renewal and proposals for new research programs as part of the field work proposal (FWP) process. These FWPs

describe past accomplishments, program milestones, and future program direction. Discussions of these proposals with OHER program managers throughout the year and the subsequent funding allocations, serve as a metric for PNL research program accomplishments and approval for planned research activities.

Fourth, throughout the year PNL reviews the research programs using a variety of peer review committees. These committees may include a standing committee (i.e., the EMSL Advisory Committee) or a one-time peer review committee assembled for a specific program review. A summary of our recent programmatic peer reviews is provided in Table 3.2. These reviews are usually accompanied by a formal report which not only provides a peer review of the scientific quality of the research but provides recommendations for future program development and growth.

Fifth, each year all staff members at PNL have a staff development review (SDR) from the laboratory line management. Each staff member is reviewed against a set of personal goals for the year and it is their performance relative to these goals that forms the basis for salary increases and promotions. For many of PNL's scientists, a major part of their staff development review is their research accomplishments for programs sponsored by the Office of Health and Environmental Research.

### 3.3 Institutional Program Development Funds

Under the LDRD Program, PNL employs discretionary funds authorized by DOE to support exploratory research and development projects. Over the years, such studies have led to successful projects of material benefit to PNL's program and OHER needs. Recent examples of such successes include projects on 1) the ARM Program and 2) development of advanced mass spectrometry and ion trapping techniques. Discretionary funding has also provided for hiring and supporting new scientific staff in advance of programmatic funding for their specific research areas.

Research responding to OHER's needs and missions is the largest single category of LDRD expenditures at PNL. This fact is indicative of the consistency of PNL's major missions with OHER's missions, and the importance that PNL places on OHER as the major supporter of its scientific base programs. Listings of LDRD projects related to OHER's areas of interest that were conducted in FY 1994 and are on-going in FY 1995 are presented in Tables 3.3 and 3.4. As noted in the tables, LDRD funding for projects related to OHER's areas of interest increased by approximately \$700,000 from FY 1994 to FY 1995. In both years, this funding represented over 40 percent of PNL's total LDRD funding.

LDRD funds range from modest expenditures for the innovative work of individual investigators to substantial support of broad new research initiatives that are responsive to OHER needs and are judged to have demonstrable growth potential. Examples of such initiatives that are directed to areas of interest to OHER include the molecular sciences research initiative, the global environmental change initiative, the microbial biotechnology initiative, and the medical systems and technology initiative.

The budgeting, approval, authorization, management, and reporting procedures for LDRD have been greatly simplified to encourage use of this resource by the most creative and productive members

of our staff. PNL's use of LDRD is limited to the exploration of new research concepts. Consistent with the requirements of LDRD, it does not include supplemental support for on-going or terminated programmatic efforts, major equipment, conferences, workshops, or seminar series; funding for these activities is obtained from other sources.

### **3.4 Compliance with Animal Welfare and Human Subjects Regulations**

All research conducted at PNL that involves the use of animal subjects is conducted in a manner that conforms with local, state, and federal laws and with DOE requirements concerning animal care and use. These activities are carefully monitored by the institutional Animal Care Committee. The Laboratory has an approved Animal Welfare Assurance State on file (Assurance Number A3353-01) with the Office for Protection from Research Risks (OPRR), National Institutes of Health (NIH). The Laboratory is also registered as a research facility under the United States Department of Agriculture Animal Welfare Regulations (Registration Number 91-R-006). Full accreditation by the American Association for Accreditation of Laboratory Animal Care (AAALAC) has been maintained since 1976.

PNL maintains an Institutional Review Board (IRB), which reviews all proposals involving potential use of human subjects. The Board is constituted and has functioned in accordance with DOE regulations as stated in 10 CFR Part 745 and DOE Orders 1300.3 and 4300.2A. The former sets forth the federal policy for the protection of human subjects at DOE. The first DOE order provides implementation for human subjects policy for all DOE-funded research and non-DOE-funded research at DOE-owned, -leased, or -controlled facilities. DOE Order 4300.2A established DOE's policies, responsibilities, and procedures for authorizing and administering non-DOE-funded work performed under DOE contracts.

Although not yet adopted by the Department of Energy, 45 CFR 46, Subparts B, C, and D are also considered by the IRB when appropriate. These subparts contain additional safeguards for specific protected classes of human subjects, i.e., fetuses, pregnant women, human in vitro fertilization, prisoners, and children.

**Table 3.3. FY 1994 - Laboratory Directed Research and Development Projects Relevant to the OHER Program at PNL**

<b>Project Title</b>	<b>Principal Investigator</b>	<b>FY 1994 Budget (\$K)</b>
<b>Environmental Sciences Research Center</b>		
Integration of Molecular Research With Environmental Phenomena	RE Wildung	63.2
<b>Global Environmental Change Initiative</b>		
A Framework for Integrating Global Environmental Change Technologies Across Multiple Spatial and Temporal Scales	LW Vail	51.8
A Multidisciplinary Investigation of Heterogeneous Atmospheric Processes	RD Saylor	236.9
Developing Capability for Global Studies to Anticipate Changes in Vegetative Cover	NJ Rosenberg	52.0
Graphical Interface for Ocean Global Circulation Models	DW Denbo	10.9
Integrated Climate Change Analyses: A Pilot Study	MJ Quadrel	85.8
Integrated Regional Climate Change	SJ Ghan	158.1
Integrated Systems Ecology as an Approach for Unifying Global Change Issues	EJ Rykiel	206.3
North American 3E Model	JA Edmonds	175.7
Spectral Mapping of the V4 Band and Determination of the Molecular Constraints for the Chlorine Nitrate Molecule	SW Sharpe	63.8
Technological Response	WB Ashton	122.1
Uncertainty Analysis for Computer Models	AM Liebetrau	58.4
<b>Medical Systems and Technologies</b>		
Ultrasonic Measurement of Elastic Properties of Bone	GJ Posakony	15.5
<b>Microbial Biotechnology Initiative</b>		
Dynamics, Modeling and Redesign of Microbial Proteins	RL Ornstein	126.5
Enzymology of Bacterial Metal Reductase and Dehalogenase	Y Gorby	149.1
Functional Characterization of Bacterial Plasmids	JK Fredrickson	60.9
Kinetics, Scale-up and Demonstration of Uranium Bioprecipitation Technology	MJ Truex	83.1
Microbial Genomics	JD Saffer	251.0
<b>Molecular Sciences Research Initiative</b>		
Advanced Separations and Mass Spectrometry	RD Smith	210.3
Bonding and Structure of Organic Ligands at Oxide/Water Interfaces	DM Friedrich	109.2
Characterization of Structure and Dynamics of Surface Adsorbates and Their Surfaces	PD Ellis	123.1
Collaborative Environment Prototype for Molecular Science	RT Kouzes	108.4
Elastic Properties, Solution Chemistry and Electronic Structures of Oxides, Silicates, and Carbonates	AC Hess	150.7
Electronic Information Space for Molecular Science Research	DM DeVaney	21.8
Environmental Catalysis	AC Hess	43.3
Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy Data Acquisition and Modeling	RT Kouzes	116.8
High Field NMR and NMR Imaging	GP Drobny	122.3



Table 3.3. (contd)

Project Title	Principal Investigator	FY 1994 Budget (\$K)
Identification and Structural Determination of Paramagnetic Species Using Pulsed EPR	MK Bowman	79.6
Magnetic Resonance Spectroscopy	HM Cho	220.8
Multinuclear Solid State NMR Characterization of Early Forms of Mineralization	PD Ellis	110.6
NMR Studies of Altered-DNA/Protein Complexes	MA Kennedy	99.0
Structural and Kinetic Studies at Model Oxide Surfaces	BD Kay	305.8
Tumor Formation in Cells and Tissues Studied by Means of Liquid-State and Solid State NMR	RA Wind	50.8
X-Ray Adsorption Fine Structure	SM Heald	415.8
<b>Director's Awards for Excellence</b>		
Physiologically Based Pharmacokinetic Modeling of Organic Waste Site Chemicals	KD Thrall	28.8
Properties of Soft X-Ray Absorption	LA Braby	61.6
<b>Grade V S&amp;E Projects</b>		
Advanced Biomedical Science and Modeling	RW Weller	113.6
Improved Analytical Ion Trapping Methods	SA Hofstadler	90.6
<b>Basic Life Sciences Initiative</b>		
Computer Modeling of DNA Perturbations	JH Miller	74.8
Fourier Transform EPR Studies of Radiation-Induced Structural Alteration of DNA	MK Bowman	85.5
NMR Studies of DNA Structure Associated With Chemical Adduction	MA Kennedy	68.9
Protein Structure Analysis	RJ Douthart	10.2
Site Specific DNA Damage by Radiation and Chemicals	BD Thrall	79.0
Spectroscopy Techniques for Analysis of DNA Damage	AF Fuciarelli	76.0
Structural Studies of Modified Histone Species	DL Springer	100.9
<b>Health Protection Standards for Hazardous Chemicals Initiative</b>		
Health Protection and Standards for Hazardous Chemicals	BL Harper	137.9
PBPK-Based Breath Analysis Instrumentation Demonstration	KD Thrall	93.8
<b>Center-Level Projects</b>		
Bonding and Structure of Organic Ligands at Oxide/Water Interfaces	CC Ainsworth	35.0
Chemical Dosimetry	G Akabani	15.9
Development of a Chemical Carcinogenic Risk Calculation Program	MF Jarvis	12.2
Ethical, Legal, and Social Implications of the Human Genome Project for Screening, Monitoring, and Health Surveillance of DOE Workers	LE Sever	14.3
Human Metabolic Parameter Development for PBPK-Based Breath Analyzer Model	RD Stenner	16.7
Physiologically Based Pharmacokinetic Modeling of Hazardous Chemicals	TE Hui	53.1
Prototype a Collaborative Scientific Work Environment	DR Adams	55.4
Real Time Dosimetry for Therapeutic Radiation Delivery	RA Craig	29.0

**Table 3.3. (contd)**

<b>Project Title</b>	<b>Principal Investigator</b>	<b>FY 1994 Budget (\$K)</b>
Synthesis of Site-Specific Lesions	DL Springer	62.6
Testing of Noise and ELF Instruments for RF/MW Interference	MH Smith	20.0
The Effect of Individual Alpha Particle Tracks on Expression of Regulatory Proteins in Individual Cells	NF Metting	94.6
Use of Proliferating Cell Nuclear Antigen Assay to Quantify Cell Proliferation in Respiratory Tract of Rodents Inhaling Chemicals or Radioactive Materials	RA Renne	4.7
<b>Total</b>		<b>5,694.5</b>

**Table 3.4. FY 1995 - Laboratory Directed Research and Development Projects Relevant to the OHER Program at PNL**

<b>Project Title</b>	<b>Principal Investigator</b>	<b>Estimated Funding (\$K)</b>
<b>Energy Technology Development Initiative</b>		
Light at Night	RG Stevens	100.0
<b>Global Environmental Change Initiative</b>		
A Multidisciplinary Investigation of Heterogeneous Atmospheric Processes	RD Saylor	300.0
Beyond Reduced Form Climate Model	DC Bader	50.0
Ecological Modeling of Regional Responses to Global Change	EJ Rykiel	350.0
Integrated Climate Change Analyses: A Pilot Study	MJ Quadrel	35.0
North American 3E Model	JA Edmonds	85.0
Uncertainty Analysis for Computer Models	AM Liebetrau	35.0
<b>Medical Technologies and Systems</b>		
Adaptive Life Simulator	LJ Kangas	50.0
Bioactive Coatings and Composites for Orthopedic Devices	AA Campbell	35.0
Detection of H. Pylori Infection Using Laser Breath Analysis Instrumentation	JJ Toth	50.0
Medical Imaging 3D Reconstruction and Visualization	RW Heiland	20.0
Optical In Vivo Blood Characterization and Multivariant Analysis	KA Stahl	40.0
Quantitation of Hypoxic Cells	AF Fuciarelli	50.0
Real-Time Dosimetry for the Delivery of Therapeutic Radiation Delivery	M Bliss	35.0
Ultrasonic Measurement of Elastic Properties of Bone	GJ Posakony	40.0
<b>Microbial Biotechnology Initiative</b>		
750 MHz NMR Determination of the 3D Structure of a Unique Reductive Dehalogenase	MA Kennedy	100.0
Dynamics, Modeling and Redesign of Microbial Proteins	RL Ornstein	225.0
Enzymology of Bacterial Metal Reductase and Dehalogenase	Y Gorby	150.0
Functional Characterization of Bacterial Plasmids	JK Fredrickson	75.0

Table 3.4. (contd)

Project Title	Principal Investigator	Estimated Funding (\$K)
Identification, Purification and Characterization of the Reductive Dehalogenase of <i>Desulfomonile tiedjei</i> DCB01	L Xun	150.0
Isolation and Use of Extremophilic Bacteria for the Treatment of High Nitrate and Sulfate Containing Wastes	BM Peyton	105.0
Kinetics, Scale-up and Demonstration of Uranium Bioprecipitation Technology	MJ Truex	100.0
Microbial Gene Expression and Genetic Engineering	JD Saffer	50.0
Microbial Genomics	JD Saffer	200.0
Microbial Informatics	RJ Douthart	125.0
Microbiological Controls on Contaminant Behavior	RE Wildung	120.0
<b>Molecular Sciences Research Initiative</b>		
Application of Mass Spectrometry to Life Science and Bioremediation Research	RD Smith	100.0
Bonding and Structure of Organic Ligands at Oxide/Water Interfaces	DM Friedrich	125.0
Characterization of Structure and Dynamics of Surface Adsorbates and Their Surfaces	PD Ellis	190.0
Collaborative Environment Prototype for Molecular Science	RT Kouzes	180.0
Environmental Catalysis	AC Hess	70.0
Evaluation of Cellular Response to Insult	CG Edmonds	100.0
Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy Data Acquisition and Modeling	RT Kouzes	75.0
High Field NMR and NMR Imaging	GP Drobny	25.0
High Resolution and Solid State NMR Studies of Proteins and DNA-Adducts	GP Drobny	75.0
Identification and Structural Determination of Paramagnetic Species Using Pulsed EPR	MK Bowman	112.0
Magnetic Resonance Spectroscopy	HM Cho	130.0
Magnetic Resonance Spectroscopy Studies of Glasses, Minerals and Catalysts	HM Cho	120.0
Multinuclear Solid State NMR Characterization of Early Forms of Mineralization	PD Ellis	124.0
NMR Studies of Altered-DNA/Protein Complexes	MA Kennedy	100.0
NMR Studies of Proteins	PD Ellis	150.0
Protein-DNA Complexes: Dynamics and Design	RL Ornstein	150.0
Tumor Formation in Cells and Tissues Studied by Means of Liquid-State and Solid State NMR	RA Wind	82.0
X-Ray Adsorption Fine Structure	SM Heald	400.0
<b>Director's Award for Excellence</b>		
Adsorption on Fe-(hydr)oxides Under Nonequilibrium Conditions	CI Steefel	25.0
Development of High-Sensitivity Detection Techniques for the Measurement of Ionizing and Non-ionizing Radiation	JC McDonald	25.0
Development of Meso-Level Perspectives for Modeling the Global Environmental Consequences of Human Behavior	SF Rayner	100.0

Table 3.4. (contd)

Project Title	Principal Investigator	Estimated Funding (\$K)
<b>Grade V S&amp;E Projects</b>		
Advanced Biomedical Science and Modeling	MR Sikov	120.0
Improved Analytical Ion Trapping Methods	RD Smith	110.0
<b>Enzymatic Processing - Basic Life Sciences Initiative</b>		
Fourier Transform EPR Studies of Radiation-Induced Structural Alteration of DNA	MK Bowman	88.0
NMR Studies of DNA Structure Associated With Chemical Adduction	MA Kennedy	85.0
Structural Studies of Modified Histone Species	DL Springer	50.0
<b>Health Protection Standards of Hazardous Chemicals Initiative</b>		
Cell and Tumor Growth Kinetics	LB Sasser	116.0
Cell Signaling Mechanisms	BL Thrall	142.0
Comparative Metabolism and Pharmacokinetics	RJ Bull	39.0
Direct and Indirect Genotoxic Mechanisms	DL Springer	89.0
Health Risk Assessment Standards	BL Harper	29.0
PBPK-Based Breath Analysis Instrumentation	KD Thrall	113.0
Technical Analysis and Integration of Health Effects Data	RJ Bull	77.0
<b>Center-Level Projects</b>		
Bonding and Structure of Organic Ligands at Oxide/Water Interfaces	CC Ainsworth	35.0
Capillary Neutron Focusing for Boron Neutron Capture Therapy	AJ Peurrung	40.0
Ethical, Legal and Social Implications of the Human Genome for Genetic Screening of DOE Workers	LE Sever	25.0
Physiologically Based Pharmacokinetic Modeling of Organic Waste Site Chemicals	KD Thrall	59.0
Real Time Dosimetry for Therapeutic Radiation Delivery	RA Craig/M Bliss	60.0
Testing of Noise Instruments for RF/MW Interference	MH Smith	10.0
Total		6,395.0

## **4.0 Research in Progress and Major Accomplishments**

Described in this section are the program orientation and research objectives within each major program area supported by OHER funding. Significant recent accomplishments are summarized in Table 4.1. Major collaborations are noted and educational programs are also described in this section.

### **4.1 Analytical Technology (KP-01)**

This area of research is in transition. Two projects associated with the measurement science portion are being wound down. The mass spectrometry research that was funded under this activity is retooling and will be involved with future health effects research efforts.

### **4.2 Environmental Research (KP-02)**

#### **4.2.1 Atmospheric Science (KP-02-01)**

The research program at PNL advances our understanding of the local- to global-scale effects of energy-related emissions on air quality and on regional and global climate. In the Atmospheric Chemistry Program (ACP), PNL continued the analysis and interpretation of data collected in the North Atlantic Regional Experiment (NARE) during the summers of 1992 and 1993. These data give evidence of the role and exchanges between the mixed planetary boundary layer and the free troposphere on the long-range transport of energy-related emissions and their photochemical reaction products. In the ASCOT program, PNL research addresses the processes by which surface exchanges of heat, moisture, momentum, and trace gases affect local- to synoptic-scale air motions. This research is vital to understanding the interactions between air flows, pollutant transport and dispersion, and surface topographical and morphological features.

In FY 1994, the PNL Gulfstream 1 research aircraft was designated a DOE research facility. As such it is available free of charge to all ACP principal investigators. An advisory board comprising representatives from PNL's research aircraft operations team, other national laboratories, and the Environmental Sciences Division at OHER, review all requests for G-1 usage and recommend approval for use to OHER. Schedule coordination is handled by the PNL team.

The G-1 aircraft and surface-based remote sensing of the vertical thermal and dynamic structure of the boundary are important tools in our atmospheric research. These experimental measurement capabilities are balanced by a modeling component that provides an interpretive framework for analyzing field observations. By developing improved ways to simulate critical atmospheric chemical, dynamic, and thermodynamic processes, we enhance DOE's capability to assess the impact of energy-related emissions on air quality on a wide range of spatial scales.

Fiscal year 1994 was a transition year for the two DOE programs in which most PNL atmospheric research is conducted. Both the Atmospheric Studies in Complex Terrain program and the Atmospheric Chemistry Program adopted the use of external peer review to establish their scientific programs beginning in FY 1995. Pacific Northwest Laboratory was awarded seven ASCOT projects and four ACP projects for FY 1995 starts. Early in FY 1995, a major redirection of the ASCOT program called for an equally major reordering of PNL's ASCOT project priorities to accentuate the coupling of our boundary-layer meteorology and atmospheric chemistry research programs.

#### **4.2.2 Terrestrial Transport (KP-02-03)**

Terrestrial transport and ecosystem functioning and response research efforts are directed toward establishing a fundamental understanding of key chemical, biological, and physical processes and their interactions and scale of impact in subsurface systems, all essential for predicting the long-term environmental effects and fate of chemicals resulting from defense-related activities. Information on these relationships is being used to predict subsurface response to contaminants, predict and mediate human exposure to contaminants in groundwater, and as a basis for a broad range of applications in energy development, environmental restoration, and biotechnology.

The research program builds on PNL's technical strengths in geochemistry, environmental microbiology, molecular biology, hydrodynamics, geology, and computational sciences. Unique intermediate-scale and field facilities/observatory are used to examine and scale the integrated effects of basic processes, and to validate concepts and predictive models. Advanced sampling methods, statistical techniques, and models aid in scaling mechanistic research to the field, quantifying system-level responses in heterogeneous environments, and extrapolating these responses to the site and regional scales.

Research in subsurface science entails fundamental investigations to explore deep subsurface environments and to understand the complex interactions of chemical, microbial, and hydrologic processes that control contaminant behavior and offer potential for remediation. Experiments on the surface chemistry of mineral solids are providing new concepts and mathematical models to describe the abiotic reactions that control mixed-contaminant sorption and surface-catalyzed degradation. Concurrent investigations are examining the origins, distribution, and function of microorganisms isolated from deep subsurface zones; information critical to successful bioremediation. The results of metabolic studies indicate that subsurface microflora have great potential for influencing the fate of inorganic and organic contaminants, producing novel chemicals, and mitigating water pollution. In addition, subsurface exploration is providing unique insight into the depth and history of deep zones of value in mineral and energy research exploration. Multidisciplinary investigations of coupled processes are demonstrating the close interrelationship between geochemical and microbial processes and their influence on mixed-contaminant hydrologic transport. Multidisciplinary transport studies are being performed in a unique intermediate-scale experimental facility, and in the field to quantitate and scale the integrated effects of hydrologic, chemical, and microbial processes on contaminant transport in heterogeneous media.

**Environmental Science Research Center.** As part of DOE's Subsurface Science Program (SSP), the Environmental Science Research Center (ESRC) helps provide the scientific basis for understanding

and restoring contaminated subsurface environments at DOE sites by developing cooperative basic research with other national laboratories, universities, other DOE components, such as DOE/EM, and the private sector. Exploratory research investments help establish new scientific concepts and multidisciplinary teams as a basis for new SSP initiatives, such as the origins of environmental microorganisms and subsurface heterogeneity. A technology transfer program helps ensure that the results of research are available for a broad range of applications, but focusing on restoration of subsurface substances impacted by ground-disposal of wastes.

Fundamental research in other parts of the SSP is being augmented and selectively linked with advanced scientific facilities and resources to provide new insights into natural phenomena needed to describe and remediate mixed contaminant behavior. Basic research is being extended to a first-principle evaluation of new concepts, understanding how chemical, microbial, and physical processes are coupled and scaled to the heterogeneous subsurface system. The new concepts are being evaluated using a combination of theory, modeling, and the iterative laboratory, intermediate-scale, and field experimentation used in other parts of the SSP. Thus, the ESRC occupies a special role in this program by

- conducting exploratory research to develop concepts and multidisciplinary research teams needed for understanding and remediating DOE mixed-waste contamination in situ, taking advantage of natural subsurface phenomena
- augmenting laboratory, intermediate-scale, and field research to aid DOE laboratories, universities, and industry in resolving problems of interactive and complex phenomena (e.g., chemistry-microbiology) and scaling (from the molecular to field levels) that are major impediments to developing and evaluating predictive and remedial action concepts
- developing advanced sampling, geostatistical, and modeling concepts and procedures to better define subsurface heterogeneity and mixed-contaminant behavior in subsurface systems at DOE sites
- establishing a strong outreach program to involve universities in subsurface science
- transferring technology that originates from national scientific programs to other DOE sites, other federal agencies, and industry.

#### **4.2.3 Ecosystem Functioning and Response (KP-02-04)**

An important part of this program is research on ecosystem dynamics in arid lands. The purposes of PNL's arid land sciences program is to understand interrelationships between abiotic and biotic components and to use this information to provide a better understanding of both natural and energy-related disturbances.

Other studies are under way for the Department of the Army. Work on the Yakima Training Center is being conducted in support of the DoD training command. Remote sensing, primarily through satellite imagery, is being used to detect and quantify environmental change resulting from

direct damage to lands from training, disturbance from secondary processes such as fire and erosion, and the response of lands to restoration. Maps are being updated for Geographic Information System (GIS) computer stations at the Yakima Training Center concerning road locations and condition, land-cover disturbance, recovery trends, fire maps, and land-slope maps.

Sage grouse habitat quality analyses are being conducted to aid natural resource managers in protecting sensitive species while permitting the Army to complete its training mission. Those analyses use newly developed methods that rely on remote sensing, GIS quantitative statistical analyses, and ecological interpretation.

**Hanford Environmental Research Park.** DOE's Hanford Environmental Research Park provides land, laboratory facilities, and a secure place for conducting environmental research. The emphasis is on coordinating and integrating the diverse educational, research, and demonstration activities that occur across the Hanford Site.

The current focus of research park activity has been to synthesize existing ecological data for publication in scientific literature and identify future research needs necessary to develop ecosystem management strategies.

### **4.3 Health Effects (KP-03)**

#### **4.3.1 Biological Research (KP-03-02)**

Biological research is addressed through a multilevel approach incorporating studies from the molecular to whole-animal levels. Emphasis is placed on gaining a quantitative understanding of dose-effect relationships and mechanisms that underlie the effects of radiation and chemicals using integrated dosimetric, molecular, genetic, cellular, and experimental-animal approaches. The ultimate objective is to identify the cause of, and to predict human susceptibility to, disease states induced by exposure to radiation or toxic chemicals. In FY 1994, mechanistic studies of DNA damage, mutagenesis, chromosome aberrations, and tumor initiation were investigated using in vivo and in vitro molecular and cellular systems and specific gene targets. These studies included analysis of the effects of exposure to radon progeny, alpha particles, chemical carcinogens, and chemicals and radiation associated with waste cleanup of nuclear sites.

**Genetic Susceptibility.** Identification of the genetic contribution to disease processes has evolved as a major thrust in FY 1994. A new project has been initiated to determine the genes responsible for susceptibility to lung tumors induced by radon. Genetically distinct, inbred rodent strains differ both in spontaneous cancer incidence as well as sensitivity to carcinogen-induced cancer, providing an ideal model system for these types of studies. At least three loci are believed to specifically modulate the pathogenesis of spontaneous and chemically-induced lung neoplasms in mice. The genes responsible for sensitivity to radon-induced lung cancer are likely to overlap the set of genes identified in the prior work. Radon-induced tumors are distinct from spontaneous and chemically-induced tumors, both in histology and rate of appearance; hence it is likely that some of the genes responsible for radon sensitivity will be unique to that system. Work to date has now shown that A/J and C57BL/6J mice do



indeed have a differential sensitivity to radon-induced lung tumors. Future studies will be designed to identify the genes responsible for that differential susceptibility and to molecularly clone those genes.

Another aspect of genetic susceptibility is the sensitivity of individuals to DNA damage. The final state of DNA damage is determined by the sensitivity to initial damage events and rate of repair of that damage. Building on the successful OHER-supported program in early events of DNA damage, work is now proceeding to address key questions in genetic susceptibility. Cell lines with differential sensitivity to initial damage and cell lines with differential ability to repair DNA damage are being examined to define the critical steps that lead to overall genetic susceptibility.

**Structure/Function Studies Related to Mechanisms of Carcinogenesis.** A widely accepted model of the molecular basis of carcinogenesis suggests that the transition from benign to malignant phenotype requires the accumulation of genetic damage in several oncogenes and tumor suppressor genes. We are concentrating our attention on defining the mechanisms of mutation and other kinds of genetic damage. These studies include investigation of the biochemistry of DNA damage, the relationship between chromatin structure and damage, and the repair of these lesions as a function of the altered DNA structures. This research is strongly linked to physical studies in the radiological and chemical physics subprogram and research at PNL that relies heavily on the new EMSL experimental and computational capabilities. This collaborative research is applying new molecular structure research methods to address the most fundamental issues in radiation and chemical carcinogenesis.

Benzo[a]pyrene diol epoxide (BPDE), a prototype polycyclic aromatic hydrocarbon, forms a number of covalent modifications to DNA that impede the progression of polymerases. Recent work with this system has shown that the repair of this damage is tightly linked to the transcriptional activity of the region. Future studies will focus on the role chromatin structure plays in this process.

The interaction of cellular and genetic damage induced by low- and high-LET radiation with damage produced by chemicals is being studied to identify health risks associated with the nuclear industry and nuclear waste sites. No interaction occurred between cellular damage induced by two of the organic solvents associated with waste cleanup (tributyl phosphate and isobutyl ketone) and damage from low-LET radiation. This finding suggests that these are not genotoxic agents and would play little role in cancer initiation after accidental exposures alone or in combination with radiation. Incorporation of mutated oncogene *K-ras* into the liver of mice combined with exposure to internally deposited  $^{239}\text{Pu}$  resulted in a marked synergistic effect for both life shortening and the induction of liver cancer. Damage from the organic solvent  $\text{CCl}_4$  did not alter tumor incidence when combined with the mutated oncogene.

**Radon Research.** In addition to the genetic susceptibility issue described above, work is being carried out to develop a fundamental understanding to allow prediction of the risks of exposure to low levels of inhaled alpha-emitting radionuclides. Analysis of data from the large-animal experiments is being concluded and the program has refocused on cellular and molecular biology. PNL's unique capabilities for single-cell radiation using the microbeam apparatus and for exposing cells in culture to radon provide a foundation for these new directions in the research of high-LET radiation. The

molecular and cellular research specifically addresses the role of oncogenes and tumor suppressor genes in radon-induced cancers, the cell proliferation kinetics and cell cycle regulation, and the effects of radon exposure on DNA as well as on DNA repair processes.

A single-cell gel (SCG) electrophoretic technique has been developed that measures DNA strand breaks based on increased electrophoretic migration out of lysed cells embedded in the middle layer of a three-layer gel formed on a microscope slide. The SCG technique has been used successfully to estimate the percentage of cell nuclei hit by alpha particles during irradiation with an in vitro radon exposure system, and to verify the hit-probability calculations of the PNL dosimetry model. The potential use of capillary electrophoresis-mass spectrometry at the single-cell level for ultrasensitive characterization of cellular components is being explored.

**Plutonium Research.** The final data collection and analysis are nearing completion for the studies on the life-span dose-effect relationships of inhaled plutonium in beagle dogs and rats at dose levels comparable to the current maximum permissible level of exposure for a radiation worker. This information will enhance our understanding of the health effects risk of low-level plutonium exposures. Comparison of the dose-response data obtained in rats and dogs exposed to plutonium and radon will facilitate extrapolating risk estimates to humans for alpha emitters.

**National Radiobiology Archives.** This project, begun in 1990, maintains for future analysis individual animal dose-effect data in a computerized database. Information on about 50,000 mice and beagles exposed to radiation (usually via internal deposition) and followed for life is available for distribution on diskette. Additional information is being archived each year. The project also includes a specimen archive of histopathology preparations from the animals. A major expansion of activities is under way as emphasis shifts from the well-defined, relatively limited beagle studies to the much larger rodent studies.

#### 4.3.2 Radiological and Chemical Physics (KP-03-03)

Studies in radiological and chemical physics focus on understanding and quantifying the fundamental processes of energy deposition by ionizing radiation, and the subsequent transport and degradation of that energy leading to biochemical and biological damage expressed at the cellular level. Emphasis is on the development of a quantitative understanding of the effects of radiation quality, dose, and dose rate on the production and repair of damage in biological systems. Basic studies in radiation physics and biochemistry are coordinated with studies in cellular and molecular biology to test fundamental concepts of radiation action. Emphasis is on relating the spatial and temporal aspects of energy deposition to the structure of biological targets, and on correlating conformational changes in critical biological molecules with damage and repair as expressed in mammalian cells.

This program includes experimental and theoretical determination of cross sections needed to understand the interaction of fast charged particles (representative of radon alpha particles and recoil particles produced in energy loss by fission and fusion neutrons in tissue) with biologically relevant materials; measurements and computer simulation of the track structure of fast charged particles used in microbeam and other radiobiological experiments; and mathematical modeling of the conformation

of DNA damage, and the interaction of lesions with repair enzymes. These studies of radiation action are designed to address basic mechanisms at an increasingly fundamental level.

Theoretical studies of DNA damage and repair in this program are closely linked to the development of new capabilities in the EMSL project. Methods, such as electronic structure calculations, molecular dynamics simulation, and Monte Carlo sampling of conformation space, are being used to model the interaction between perturbed DNA sequences and repair enzymes. The nuclear magnetic resonance facilities in the EMSL provide a firm experimental basis for this modeling activity. The planned expanded NMR capabilities of the EMSL will provide a unique opportunity to gain solution-phase structural data on damaged DNA complexed with repair enzymes.

The biological consequences of irradiation begin with energy deposition and transport in condensed-phase materials. Data have been obtained for electron emission from condensed molecules, frozen on the surface of thin substrates as a result of the passage of energetic protons. In these measurements, the energy and angular distributions of emitted electrons provide detailed data for testing Monte Carlo models developed to describe energy transport and charged-particle track structure in condensed-phase media. These models describe the initial densities of energy deposition by high-LET radiation and provide the basic physics for interpretation of the relative biological effectiveness (RBE) of high-LET radiation.

## **4.4 General Life Sciences (KP-04)**

### **4.4.1 Structural Biology (KP-04-02)**

A new program was initiated in FY 1993 to model structure-function-dynamic relationships in cytochrome P450 enzymes, with a goal of redesigning these enzymes for a variety of applications in bioremediation and biotechnology. Starting from a structure determined by x-ray crystallography, molecular dynamics simulations are being performed on crystal complexes and docked native and non-native substrates in the enzyme active site. Predictions are then made on the effects of modifications in the enzyme active site on substrate specificity and catalytic efficiency. Site-directed mutagenesis procedures are being used to genetically engineer enzymes with modified active sites, followed by tests to determine the resultant changes in catalytic functionality. The procedures are initially being carried out with the P450 camphor enzyme system and haloalkane (1,2-dichloroethane) dehalogenase, which is being redesigned to achieve regiospecificity for native substrate analogs and various halogenated hydrocarbons. Exploratory research is also being conducted to understand fundamental structure-function-dynamic relations of enzymes in chemically and physically harsh environments, in order to be able to redesign enzymes for improved bioremediation directly under environmentally relevant harsh conditions.

### **4.4.2 Genome (KP-04-04)**

We plan to develop electrospray ionization mass spectrometry (ESI-MS) methods for high-speed DNA sequencing of oligonucleotide mixtures, that can be integrated into an effective overall sequencing strategy. Electrospray ionization produces intact molecular ions from DNA fragments of

different size and sequence with high efficiency. Our intent is to determine mass spectrometric conditions that are compatible with biological sample preparation and that avoid problems due to dissociation, aggregation, or adduction of the ionized DNA fragments. Oligonucleotide ions are typically produced from ESI with a broad distribution of net charge states for each molecular species (i.e.,  $(M-nH)^n$ , where  $n$  is a series of integers), and thus leading to difficulties in analysis of complex mixtures. To make identification of each component in a sequencing mixture possible, the charge states of molecular ions can be reduced by manipulating the ESI process and/or by using gas-phase reactions. The charge-state reduction methods being examined include 1) reactions with organic acids (in the solution to be electrosprayed, the ESI-MS interface, or the gas phase); 2) labeling of the oligonucleotides with a designed functional group for production of molecular ions of very low charge states; and 3) shielding of potential charge sites on the oligonucleotide *phosphate/phosphodiester* groups with polyamines (and the subsequent gas-phase removal of the neutral amines). In initial studies, two methods for charge state reduction of gas phase oligonucleotide negative ions have been tested: 1) the addition of acids to the oligonucleotide solution and 2) the formation of diamine adducts followed by dissociation in the interface region. In the first method, the efficiency of charge state reduction depends on the  $pK_a$ , the concentration, and the nature of the acids. Acetic and formic acids were found to be better reagents than HCl,  $CF_3CO_2H$ , and  $H_3PO_4$ . The second method has the advantage that the stability of oligonucleotides is not affected but requires the optimization of the interface dissociation conditions and the amounts of diamine added to the oligonucleotide solution. Both methods show promise for charge state reduction and results have been demonstrated for small oligonucleotides (e.g.,  $pd(T)_{12}$  and  $d(AGCT)$ ). Substantial reduction in spectral complexity was also observed for a four-component mixture of oligonucleotides upon charge state reduction. Our aim is to provide a basis for the development of an overall approach to high-speed sequencing so as to provide a basis for the subsequent step of prototyping a cost-effective high-throughput instrument for broad application.

Another part of this project is directed at the development of a totally new concept for high speed DNA sequencing based on the analysis of single (i.e., individual) large DNA fragments using ESI combined with Fourier transform ion cyclotron resonance (FTICR) mass spectrometry. In our approach, large single-stranded DNA segments extending to as much as 25 kilobases (and possibly much larger) are first transferred to the gas phase using ESI. The multiply-charged molecular ions are then trapped in the cell of an FTICR mass spectrometer, where one or more *single ion(s)* can be selected for analysis and its mass-to-charge ratio ( $m/z$ ) measured both rapidly and nondestructively. Single ion detection is achievable due to the high charge state of the electrosprayed ions.

Our efforts during the first two years of this project have demonstrated the capability for the formation, extended trapping, isolation, and monitoring of sequential reactions of highly charged DNA molecular ions with molecular weights well into the megadalton range. We have shown that large multiply-charged individual ions of both single and *double-stranded* DNA anions can also be efficiently trapped in the FTICR cell, and their mass-to-charge ratios measured with very high accuracy. Thus, it is feasible to quickly determine the mass of each lost unit as the DNA is subjected to rapid reactive degradation steps. We plan to develop methods based on the use of ion-molecule or photochemical processes that can promote a stepwise reactive degradation of gas-phase DNA anions. Successful development of one of these approaches could greatly reduce the cost and enhance the speed of DNA sequencing, potentially allowing for sequencing *DNA segments of more than 25 kilobases* in length, on

a time-scale of minutes with negligible error rates, with the added potential for conducting many such measurements in parallel. *The techniques* being developed promise to lead to a host of new methods for DNA characterization, potentially extending to the size of much larger DNA restriction fragments (> 500 kilobases).

## 4.5 Global Change Research Program (KP-05)

As an integral component of the U.S. Global Change Research Program developed by the Committee on Earth and Environmental Sciences, DOE's Global Change Research Program at PNL is focused on the following areas:

- the measurement and parameterization for computer modeling of the effects of greenhouse gases and clouds on radiative transfer through the atmosphere
- the development of models for predicting future emissions of greenhouse gases
- research into processes responsible for the exchange of greenhouse gases between the atmosphere and oceans and for the transport of mass, momentum, and heat between the surface and deep layers of the ocean
- the development of improved physical process modules for the next generation of global climate models
- the development of new technologies for measuring CO<sub>2</sub> in seawater.

These areas emphasize research that is needed to improve our ability to forecast the effects of continuing emissions of greenhouse gases on the Earth's climate system.

Radiative transfer processes in clear sky and in the presence of clouds are the focus of the ARM Program, a DOE initiative to improve the reliability of predicting the regional and global climate changes resulting from increasing atmospheric concentrations of greenhouse gases, including CO<sub>2</sub>. Cloud radiative feedbacks are being studied with the aid of advanced instrumentation on the ground and on new airborne and space platforms. ARM is a multilaboratory effort with the Program Office located at PNL. The experimental infrastructure of ARM, known as the Cloud and Radiation Testbed (CART), provides the ability to deploy advanced measurement systems, to test subgrid-scale process models, and to integrate the observational program with the scientific goals of ARM. As the manager of ARM for DOE, PNL is responsible for coordinating and integrating the field and laboratory measurement programs, modeling studies, and data-analysis activities within ARM. Scientists in universities, DOE laboratories, and other government agencies, recruited by a competitive, peer-review process, form a Science Team of more than 60 persons to guide ARM research.

Pacific Northwest Laboratory continues its efforts to define the historical and future trends in CO<sub>2</sub> emissions. One of the most serious uncertainties in estimating climate change and its effects is that associated with future global emissions of greenhouse gases. Establishing a scientific basis for

forecasting future emissions of CO<sub>2</sub> and other radiatively active gases as a function of time and country is an active area of research at PNL that will improve emissions forecast methods and facilitate the validation of emissions models.

Critical uncertainties in the relationship among atmospheric CO<sub>2</sub> concentrations, the oceans, and climate change are being addressed in a PNL-directed program of research on ocean-atmosphere interactions and climate change. In collaboration with scientists from universities and government, researchers at PNL are currently focusing on air-sea interactions, ocean circulations, climate and marine carbon cycle modeling, and ocean measurement technologies.

Design of the CHAMMP Program has been completed. The goal of the program is to improve the performance of global climate models by improving the representation of key model processes, and by increasing the computational throughput of the models by a factor of 10,000. A PNL staff member detailed to the Environmental Sciences Division (ESD) is providing technical guidance to the implementation of the program. Scientists at PNL's Marine Sciences Laboratory are contributing to the program objectives through the development of an improved scheme for parameterizing deep oceanic convection (i.e., deep water formation) in the next generation of ocean general circulation models (OGCMs).

Recent work at PNL in collaboration with colleagues at EPRI and the University Corporation for Atmospheric Research has focused on a better understanding of the implications of the Framework Climate Change Convention. Edmonds, Richels, and Wigley have developed a set of fossil fuel carbon emissions trajectories which are associated with alternative ceilings of atmospheric carbon dioxide and minimal economic cost of adjustment for the global energy system. These trajectories will appear in the *Second Assessment Report of the Intergovernmental Panel on Climate Change*. Edmonds, Richels, and Wigley's work draws upon both economic and natural science and highlights the value of integrated assessment modeling. They have drawn three important lessons: 1) in the portfolio of actions invoked to comply with the ceiling, measures which lead to premature retirement of existing capital infrastructure should be avoided except in extreme circumstances; continued growth in emissions for the next 20 years may be consistent with atmospheric CO<sub>2</sub> ceilings as low as 450 ppmv; 2) careful consideration should be given to the characteristics of new energy using infrastructure; and 3) since to a first approximation all tons of carbon removed are alike, investments should be made early on in research to develop technologies which reduce the cost of emissions reductions in the future.

The analysis recognizes that a particular concentrations target can be achieved through a variety of emission time-paths. The economically efficient emissions profile is one that allows for an economical turnover of the existing capital stock and time to develop ample supplies of low-cost substitutes. Fortunately, concentration targets of 450 ppmv and above need not be inconsistent with the goal of economic efficiency. That is, they can still provide for a gradual transition away from carbon-intensive fuels.

These results should not be interpreted as supporting a "do nothing" policy, but rather that the future capital stock be less carbon intensive. This has important implications for current investment decisions since new supply options typically take many years to enter into the marketplace. To have

sufficient quantities of low-cost substitutes in the future will require a sustained commitment to research and development today. The focus of the analysis is on mitigation costs. As such it provides only partial guidance for policymaking. Different emission profiles yield different concentration levels in the years leading up to a particular concentrations target. The implications for damages need to be considered. Unfortunately, the knowledge base is not yet available to prepare an optimal strategy considering the full array of costs and benefits.

## 4.6 Medical Applications (KP-06)

Pacific Northwest Laboratory's biomedical program places a strong emphasis on the development of new imaging, biosensing, and computational technologies for medical applications.

Another component of this program is the production of new radioisotope products for the diagnosis and treatment of disease, and the development and application of quantitative dosimetry procedures for estimating the radiation doses delivered to tumors and other body regions by radiolabeled monoclonal antibodies.

Medical imaging research is focused on the reconstruction of information obtained by nonionizing modalities such as fluorescence signals, infrared imaging, ultrasound holography, and the mapping of magnetic and electric signals from the brain. In sensor technology, a breath analysis instrument has been developed that can be coupled to a mass spectrometer for detecting metabolites of ingested drugs or toxic chemicals. Sensor systems are also under development for the real-time monitoring of radiation exposure during tumor treatment by conventional radiotherapy or by an experimental procedure involving boron-neutron capture therapy. In computational medicine, PNL is developing cost-effective tools for medical image visualization, diagnostic assistance and information processing, and telemedicine. The telemedicine program includes development of telerobotic systems that enable remote operations to be performed through the use of high-bandwidth communication and three-dimensional workspace mapping.

The medical isotopes program involves the development of radiolabeled tumor-targeting molecules for the selective administration of high radiation doses to tumors. PNL currently produces most of the yttrium-90 being used at six cancer centers throughout the United States for the treatment of several major types of cancer, including leukemia, lymphomas, breast tumors, lung tumors, ovarian cancer, brain cancer, and prostate tumors. The results of initial therapy trials using radiolabeled monoclonal antibodies against Hodgkins lymphoma have been remarkable, with remissions being observed in 80% of the patients treated to date by this procedure. PNL is also providing medical internal radiation dosimetry support to Phase 1 and Phase 2 clinical trials using radiolabeled antibodies at several major cancer centers, including the University of Washington Medical Center, the Fred Hutchinson Cancer Research Center, the Virginia Mason Cancer Clinic, and the Louisiana State University Medical Center.

## **4.7 Academic and Minority Programs**

### **4.7.1 Science Education Center Programs**

Pacific Northwest Laboratory conducts a strong and aggressive program for students and faculty in elementary and secondary schools, and in community colleges. During FY 1994, PNL's Science Education Center hosted 141 elementary, middle, and high school teachers, and 73 high school and community college students in laboratory research appointments. Forty-eight students and 62 teachers participated in research activities related to OHER programs.

Under the Teacher Research Associates (TRAC) program, PNL researchers working on OHER programs assisted teachers in studies related to marine sciences, wetland ecology, microbiology, terrestrial sciences, global environmental change, geosciences, computer modeling, molecular biology, cell biology, inhalation toxicology, and wildlife studies on the Fitzner/Eberhardt Arid Lands Ecology Reserve. The TRAC program is conducted by PNL's Science Education Center and is administered through Associated Western Universities (AWU).

Pacific Northwest Laboratory researchers in areas related to OHER dedicated a total of 1079 hours in FY 1994 to working with students and teachers in elementary and middle schools in the Yakima Valley area having large populations of traditionally underutilized ethnic populations. They participated in PNL OPTIONS and Science Alive programs. These programs are part of the DOE/PNL initiative in the Northwest to revitalize sciences, mathematics, and technology education.

Ten Washington State high school students participated in marine ecology research at PNL's MSL in Sequim. The program, involving OHER researchers, was part of the 1994 High School Student Workshops sponsored by the Centrum Foundation of Port Townsend, Washington. Student studies included estuarine, intertidal, nearshore, and field and forest studies of animals and plants as well as water quality issues, marine toxicant studies, and marine organism pathology.

Under PNL's Sharing Science with Schools Program, PNL researchers made 198 presentations reaching 9953 teachers and students in area schools, of which 40 were on topics related to OHER research at PNL.

### **4.7.2 University Programs**

Minority Programs under PNL's University Programs Office continued to support university faculty and students in the summer of 1994, with more than 45 internship appointments through PNL. The greatest growth continues to be in areas related to OHER. Memoranda of Understanding are in place with nine Historically Black Colleges and Universities to facilitate these activities.

More than 150 PNL staff members involved in OHER programs hold adjunct appointments at regional universities, and approximately 200 faculty members from universities nationwide are involved in research at PNL in either full-time or part-time capacity.



University Programs at PNL operates undergraduate, graduate, and faculty research programs for the DOE in association with Associated Western Universities, Northwest (AWU-NW). Associated Western Universities, Northwest is an association of schools and industries, and provides administrative support for DOE research appointments at PNL in science, engineering, and mathematics. Under PNL's DOE University/Laboratory Cooperative Program, approximately 500 undergraduate and graduate science and engineering student appointments and 250 faculty and postdoctoral internships were granted in FY 1994. These internships in OHER-related research included graduate dissertation, research, graduate fellowships, postdoctoral appointments, summer faculty intern appointments, faculty sabbatical appointments, and faculty workshop appointments.

The DOE Science and Engineering Research Semester (SERS) Program for outstanding college juniors and seniors is administered by PNL during the academic year. During FY 1994, a majority of the 90 SERS students participated in OHER-related research.

In addition, the Office of University Programs administers projects that encourage collaboration with universities. During FY 1994, these included faculty appointments, joint research projects, scientist/faculty exchanges, and engineering and research fellowships that were related to OHER programs.

See Table 4.2 for examples of collaborative research with other OHER-supported groups. Table 4.3 lists license agreements and patents. Examples of Work for Others during FY 1995, arranged by subprogram research category, are provided in Table 4.4.

**Table 4.1. Significant Science and Technology Achievements**

Subprogram	Achievements
KP-02	<ul style="list-style-type: none"> <li>Modeling studies were used to isolate the mechanism that produces strong winds over the Hanford Site during spring and summer evenings.</li> <li>Unusual semidiurnal wind oscillations were discovered in climatological analyses of wind data obtained from a vertically-pointing Doppler meteorological radar. Our further analyses have shown that these oscillations extend through the troposphere and can be observed throughout North America. Their characteristics suggest that they are semidiurnal solar thermal tides.</li> <li>A Monte Carlo method has been developed to evaluate the energetics of atmospheric control volumes using networks of atmospheric remote sensing systems.</li> <li>A cluster analysis method was developed to categorize meteorological wind field patterns over areas of complex terrain.</li> <li>A large-scale mountain-plain circulation over and surrounding the Rocky Mountains was documented using analyses of meteorological radar data from two sites on the east and west sides of the Rocky Mountains.</li> <li>An analysis of wind data in the Swiss Mittelland (the low-lying area between the Alps and Jura Mountains) showed that wind channeling depends on the along-valley component of the large-scale pressure gradient, but is also affected by Alpine perturbations to the large-scale pressure pattern.</li> <li>Data collected with the Gulfstream-1 aircraft during 1992 and 1993 field campaigns to the western North Atlantic (WNA) established that the maximum in ozone concentrations that typically occurs above or near the top of the marine boundary layer, rather than at the surface, is a consequence of surface deposition as clean air masses move toward the WNA.</li> <li>Aircraft observations established that southwesterly flow in advance of cyclonic systems moving into the WNA is the predominant mechanism for the flux of anthropogenic pollutants into this region. The injection of anthropogenic material into the airshed of the WNA is highly episodic and shows a strong dependence on latitude.</li> <li>Optical depths simulated by the PNL Global Chemistry Model exhibited spatial patterns similar to those observed by satellite off the east coast of North America.</li> <li>The oxidation of SO<sub>2</sub> and NO<sub>x</sub> within the Kuwait oil fire plumes of August 1991 is best explained as a second-order process with conversion rates of 1% and 2% per hour, respectively, within 100 km of the oil well fires. These conversion rates are of interest to the scientific community because these constituents are closely associated with acid rain, which was of concern during wet removal outside the Persian gulf.</li> <li>Methane emissions on a global scale were estimated using a photochemical model in conjunction with full and truncated singular value decomposition as part of a project to quantify the uncertainty associated with these emissions.</li> <li>The thermodynamics and kinetics of adsorption, mineral dissolution, and metal exchange reactions that control the geochemical behavior of radionuclide-EDTA (ethylenediaminetetraacetic acid) complexes in subsurface materials have been quantified. The transport behavior of these complexes has been shown to exhibit complicated time and distance variant retardation as a result of the multiple reaction suite controlling its concentration and stability.</li> <li>Metal reducing bacteria have been shown to exert complex effects on the reactive chemical transport of radionuclide-EDTA complexes by changing the chemical properties of adsorbing Fe oxide surfaces and through evolution of FE<sup>2+</sup> which functions as a reductant and as a competitive ion for surface sorption sites and aqueous complexing ligands.</li> </ul>

Table 4.1. (contd)

Subprogram	Achievements
KP-02 (contd)	<ul style="list-style-type: none"> <li>• Spectroscopic measurements of U(VI) doped clay minerals combined with macroscopic interaction experiments of U(VI) with specimen clays and clays isolated from subsurface sediments at DOE sites have allowed development of a comprehensive surface chemical model that predicts the adsorption behavior of U(VI) to clay containing materials over a broad range of pH and other geochemical variables.</li> <li>• The pH dependence of chelate desorption rates from common mineral oxides have been determined for the first time and have important implications for chelate degradation and associated radionuclide transport. Nitilotriacetic acid (NTA) desorption from gibbsite was highly pH dependent with desorption half lives of 1, 17, and 80 hours at pH 8, 7, and 6, respectively. This is consistent with formation of inner-sphere multidentate NTA surface complexes on gibbsite.</li> <li>• Fundamental studies have shown that at DOE sites where radionuclides and NTA were co-disposed, NTA may persist for extended periods under acidic conditions because of long NTA retention times on gibbsite. Adsorbed NTA is unavailable for degradation by <i>Chelatobacter heintzii</i> at pH 6, 7, and 8. A couples process sorption-degradation model showed that the rate of NTA desorption decreases with decreasing pH. Gibbsite occurs naturally under acid conditions.</li> <li>• The <math>^{60}\text{Co}</math> added as the Co-NTA complex was primarily associated with the gibbsite with only a small fraction (i.e., 4%) associated with <i>C. heintzii</i> after NTA degradation in the presence of gibbsite. The majority of the Co would therefore be subject to cation-like adsorption to gibbsite with <math>^{60}\text{Co}</math> retardation being dominated by sorption processes. With only a small fraction of the <math>^{60}\text{Co}</math> associated with <i>C. heintzii</i> biomass, bacterial population dynamics will have little effect on <math>^{60}\text{Co}</math> transport and fate.</li> <li>• <math>^{60}\text{Co}</math> and Pu isotopes have been co-disposed with chelating agents (NTA and EDTA) and enhanced subsurface migration of chelated radionuclides has been reported at several DOE waste sites. Pacific Northwest Laboratory investigated the adsorption of CoNTA and CoEDTA on common oxide minerals occurring in the subsurface and found that the presence of EDTA completely alters the adsorption behavior of <math>^{60}\text{Co}</math> both as Co(II) or Co(III) ions. Thus EDTA can substantially affect the attenuation and transport of <math>^{60}\text{Co}</math> within the boundaries and possibly beyond the boundaries of DOE sites.</li> <li>• The kinetics of chelated radionuclide sorption-desorption has a major impact on the rate of radionuclide migration and upon chelate biodegradation rates. These in turn have a major effect on bioremediation strategies for chelate removal at co-disposal sites. Pacific Northwest Laboratory established that NTA desorption rates from common Al oxides are very slow and are highly dependent on pH, with desorption half lives of 1, 16, and 80 hours at pH 8, 7, 6, respectively. Spectroscopic and structural evidence suggests that this pH dependence is due to the enhanced formation of multidentate, inner sphere surface complexes with decreasing pH.</li> <li>• Mechanistic modeling of equilibrium and kinetically controlled sorption processes, which incorporate both molecular and macroscopic considerations, have been highly successful in describing and interpreting chelate and chelated radionuclide adsorption behavior.</li> <li>• Field sediment cores were collected using sterile methods and microbial communities were analyzed immediately by researchers at Florida State University, the University of Tennessee, and Rensselaer Polytechnic Institute. The total numbers of viable microorganisms decreased sharply with depth at both the high and low recharge sites. Analysis of microbial membrane lipids (ester-linked phospholipid fatty acids or PLFA), in particular, resulted in two interesting observations. PLFA representative of a specific class of surface soil microorganisms, the Actinomycetes, and PLFA ratios representative of increased metabolic stress of the microbial community were observed throughout the depth intervals only at the sites where high recharge occurred. The detection of tuberculostearic acid indicated the presence of the Actinomycete group of microorganisms which are typically abundant in surface soils, but usually absent in deep sediments and groundwater.</li> </ul>

Table 4.1. (contd)

Subprogram	Achievements
KP-02 (contd)	<ul style="list-style-type: none"> <li>• In sequence of Miocene-aged fluvial sediments, anaerobic sediments hosted distinct phylogenetic groups of bacteria, as determined with 16S rRNA oligonucleotide probes, with greater diversity in phylogenetic types occurring at sedimentary interfaces. Lacustrine sediments were dominated by sulfur-reducing bacteria and other delta group bacteria, consistent with observed pyrite mineralization and measured concentrations of organic carbon, dissolved sulfate, and bioavailable iron, while phylogenetic groups occurring in paleosols (alpha group and enterics in one paleosol and archaeobacters and beta group in second paleosol) and fluvial sands (enterics, plus flavo and alpha group bacteria) reflected geochemical conditions inconsistent with sulfate reduction.</li> <li>• Microbial transport was found to be unlikely through lacustrine sediments where initial pore structure and occlusion of porosity by secondary silica and clays leads to &gt;95% of pore throats being less than the size (&lt;0.8 microns) of microorganisms found in oligotrophic environments.</li> <li>• The design of effective remediation strategies depends on the ability to accurately predict the subsurface transport and transformation of contaminants in complex subsurface systems. In bioremediation, the fate of contaminants is, in part, controlled by the distribution of microorganisms in the subsurface. Previous field studies have shown that predictive ability is limited by 1) a lack of understanding of interacting processes on a mechanistic level, and 2) an inability to scale mechanistic processes from observations in the laboratory to the field. Improving our understanding of mechanistic processes and the ability to scale these processes to relevant field problems can best be addressed by controlled laboratory experimentation in intermediate-scale flow cells.</li> <li>• Intermediate-scale experiments have moved from simple layered systems to complex physical heterogeneities that approximate sedimentary formations commonly found in the eastern coastal plain and western alluvial sites. This heterogeneity pattern is described as a binary inclusive field where low-conductivity inclusions (e.g., clasts or detrital remains such as lignite) are randomly distributed in a high conductivity matrix, such as sand. High-resolution premodeling of such a field indicated that the low-K inclusions were associated with increased microbial growth. Substrate that diffused and dispersed into these low-K regions had a longer effective residence time than in the high-K material, allowing organisms in this region to metabolize a larger fraction of the substrate pulse there.</li> <li>• Experimental results show that the shape of tracer breakthrough curves is highly dependent on the variability over flow streamlines of the separation distance between inclusions. This significant result has strong implications for viable scaling methods. For instance, periodic methods, which rely on a uniform spatial distribution of heterogeneities, cannot capture this aspect of the pattern. One interesting ramification is that uniform packings of inclusive heterogeneities, which have commonly been used in previous work, may largely misrepresent transport in natural systems.</li> <li>• Parallel work on the descriptive microbial kinetics and transport physics has shown that a stochastic treatment of the heterogeneities affords separability between the scaling of the transport process and of the microbial degradation process. Specifically, a stochastic-convective reaction (SCR) method was developed which allows independent treatment of the solute transport problem from the nonlinear solute reactions such as microbial degradation with growth, abiotic chemical transformations, or sorption reactions. Complex simulations demonstrated that the SCR method more accurately predicts the upscaled coupled nonlinear reaction and transport than conventional approaches, such as the convective-dispersion equation.</li> <li>• Developed modeling approach for support of OHER/SSP planned experiments in in-situ bacterial transport in sandy aquifer near Oyster, Virginia. Research involves both deterministic high-resolution modeling and stochastic and nonlocal upscaling approaches, used to support SSP research in developing models for kinetic bacterial attachment, in designing injection experiments, and in assessing experimental outcomes and the effects of chemical and physical heterogeneities.</li> <li>• The environmental factors controlling microbial numbers and activity in subsurface sediments were studied in two vertical transects at White Bluffs, Washington. These sediments contained low microbial numbers and activities. The data suggested that microorganisms capable of metabolic activity exist as "islands" of individual cells or small microcolonies, with distances of a few centimeters between "islands." This is a distribution very different from surface soils, where distances</li> </ul>

Table 4.1. (contd)

Subprogram	Achievements
KP-02 (contd)	<p>between microorganisms capable of metabolic activity are several orders of magnitude smaller. When the sediment was moistened the microbial community was stimulated and has potential for bioremediating subsurface contaminants.</p>
KP-03	<ul style="list-style-type: none"> <li>Physical and chemical properties (permeability, porosity, silica, and extractable iron) showed spatial continuity at a range of approximately 20 cm, which was related to the average thickness of the lithologies in the transects. Microbiological variables were measured at the same sample spacing (7.5 cm) but did not show any spatial continuity. The results indicate that smaller sample separation distances may be required to detect microbiological spatial structure in these subsurface sediments.</li> <li>Developed "stochastic-convective reactive" transport model to upscale the subsurface transport of solutes that react with the solid phase (including kinetic sorption and biodegradation with coupled microbial growth). Model successfully applied to intermediate-scale experiments in transport in porous media with biodegradation.</li> <li>PNL staff have demonstrated that the appearance of radon-induced lung cancer in mice is regulated at the molecular level by mechanism that differ from those regulating chemically-induced tumor formation.</li> <li>A draft protocol for standardized analyses of experimental data from radiobiologic animal studies has been prepared. This protocol sets out the details of the statistical methods and models that are to be used in these standardized analyses.</li> <li>Analyses of data on rats exposed at PNL to radon have been completed. These analyses include recent data on animals exposed at low exposures and exposure rates, and make use of recently developed software that allows utilizing pathologists' judgments on whether tumors are fatal or incidental.</li> <li>Methods were developed to "paint" rat chromosomes which makes it possible to follow cells that have chromosome translocations associated with the development of cancer. We have also determined the best methods to culture cells from different regions of the respiratory tract so that inhaled energy effluents can be studied in relevant epithelial cells.</li> <li>The relationship between the exposure to radon to the dose to the critical cells of the respiratory tract in mGy has been established. PNL staff have gained international recognition from these studies and are using the data to help define the risk associated with radon inhalation.</li> <li>PNL researchers have demonstrated that different physicochemical forms of inhaled plutonium produce predictable stochastic (cancer) effects as well as significant deterministic (noncancer) effects. These data have been used to estimate dose and risk in human subjects, and to validate or modify dosimetry models and safety and radiation protection standards.</li> <li>Key information has been provided regarding the nature and pattern of DNA damage induced by various energy-related byproducts. This work will serve as the basis for defining differences in cellular sensitivity to physical or chemical genotoxic agents.</li> <li>PNL staff and collaborators have shown that the spectrum of DNA damage in mutations derived from radon-irradiated mammalian cells is distinctly different from that seen in mutations of spontaneous origin.</li> <li>A technique was developed for measuring electrons emitted in collisions between fast protons and biological materials in the condensed phase. This technique has produced new data on how energy is deposited and transported in biological tissues.</li> <li>We have shown that transient changes in cell cycle regulation following a single alpha particle event in the cell are similar to epigenetic effects that can lead to permanent alterations in gene regulation following x-ray irradiation.</li> </ul>

Table 4.1. (contd)

Subprogram	Achievements
KP-04	<ul style="list-style-type: none"> <li>Recent studies by Wackett and coworkers have shown that cytochrome P450cam is capable of reductively dehalogenating hexachloroethane at a significant rate, but that no appreciable dehalogenation of 1,1,1-trichloroethane (a high priority DOE pollutant) is observed. Our recent simulations suggest that differences in intrinsic reactivity cannot completely explain this observation. We have now obtained a specific double mutant of P450cam that theoretically is expected to have a much better binding constant and lead to reductively dehalogenation of 1,1,1-trichloroethane. This double mutant is currently being constructed experimentally.</li> <li>MD trajectories were calculated separately on the crystal structure of the hemoprotein domain of cytochrome P450bm3. The mouth of the substrate binding pocket is dramatically more open in the time-average MD structure. The mouth region for this enzyme molecule also undergoes large amplitude motions during the trajectory. Presumably binding of different substrates will induce the mouth region to adopt different conformations from within the wide range of structures that are accessible in the simulation. Lattice packing forces presumably prevent such motions in the crystal state.</li> <li>MD trajectories were calculated separately for open and closed active site conformations of the M6I mutant of T4 lysozyme. In the x-ray structures, the distance across the mouth of the active site ranges from 17 Å to 25 Å. The time-average structures in the simulations all converge at a value of about 17 to 18 Å. Thus lattice-packing forces appear to play a significant role in leading to observed structures. While the mouth of the active site closed in this case, the opposite effect was noted above for cytochrome P450bm3.</li> <li>The reported crystallographic structure for norcamphor-bound P450cam models norcamphor as the D-isomer. Unfortunately, the two stereoisomers have never been separated. Three simulations each of the L- and D-isomers of norcamphor bound to cytochrome P450cam were compared to account for the effects due to substrate orientation and the assignment of random velocities. The results show that the L-isomer of norcamphor is predicted to give rise to predominately 6-hydroxynorcamphor, while the D-isomer gives rise to mainly 5-hydroxynorcamphor. From this data, we infer that racemic norcamphor will give rise to non-racemic 5- and 6-hydroxynorcamphors after oxidation by cytochrome P450cam. Two years after the original prediction, the experimental results confirmed the prediction.</li> </ul>
KP-05	<ul style="list-style-type: none"> <li>A new method based upon Fourier transform ion cyclotron resonance mass spectrometry has been developed, and it has been demonstrated that intact double stranded DNA of up to 300 kbp can be studied, nearly three orders of magnitude larger than previous mass spectrometric methods.</li> <li>A new approach for high-speed DNA sequencing has been demonstrated based upon the use on ion-molecule reactions to reduce the extent of charging and sodium adduction with the electrospray ionization of mixtures of nested sets of oligonucleotides.</li> <li>An assessment conducted for the Intergovernmental Panel on Climate Change (IPCC) suggests that maximum atmospheric concentrations as low as 450 ppmv can be achieved through a policy that allows for economically efficient retirement of existing capital stock as long as it is replaced with new low or zero carbon emission technology.</li> <li>A new parameterization scheme has been developed for estimating subgrid-scale variations in precipitation that result from subgrid-scale terrain features. The scheme greatly improves the accuracy in simulating terrain-forced precipitation patterns in mountainous areas.</li> <li>Work was begun on a state-of-the-art assessment of the degree of understanding the social sciences have of the human implications of global climate change.</li> <li>Progress continued on the development of a new scheme for parameterizing penetrative deep convection in an operational climate model. A new one-dimensional parameterization scheme was successfully incorporated into the Parallel Ocean Climate Model (POCM). The new scheme improved representation of penetrative convection in a test application of the model.</li> </ul>

Table 4.1. (contd)

Subprogram	Achievements
KP-05 (contd)	<ul style="list-style-type: none"><li data-bbox="320 359 1333 436">• Acquisition of the Atmospheric Radiation and Clouds Stations (ARCS) was initiated. The ARCS are modular observing stations that will be used to make ARM measurements in the Tropical Western Pacific and the North Slope of Alaska.</li><li data-bbox="320 464 1333 596">• Analysis of data from an experiment conducted near Boardman, Oregon, shows that although large variations in surface characteristics (e.g., albedo, surface roughness, surface cover) can induce mesoscale variations in near-surface wind fields, these variations contribute very little to the vertical transport of heat, momentum and moisture. Consequently, surface exchange rates for these types of situations are dominated by small-scale turbulent transport.</li><li data-bbox="320 623 1333 730">• Analysis of wind and cloud climatology from the ECMWF model and the NCAR Community Climate Model indicates that high resolution versions of these models (resolution finer than rhomboidal truncation R15) do a credible job of representing the low level jet (LLJ) in the southern Great Plains ARM/CART site.</li><li data-bbox="320 758 1333 884">• Gas transfer data collected in experiments conducted in the whitecap simulation tanks have been used to develop a parameterization of the gas transfer velocity in terms of white cap coverate, Schmidt number, and aqueous-phase solubility. Also, concurrent measurements of passive microwave brightness temperatures and transfer velocities show a linear relationship between the two. This suggests that a remote sensing technique may be used to estimate the gas transfer velocity.</li></ul>

**Table 4.2. Collaborative Research**

National Radiobiology Archives	GE Dagle, ES Gilbert, CR Watson, JF Park, RC Thompson, JA Mahaffey, MT Karagianes, SK Smith, LG Smith, RE Weller, Pacific Northwest Laboratory (PNL) BB Boecker, BA Muggenburg, Inhalation Toxicology Research Institute (ITRI) B Carnes, TE Fritz, D Doyle, Argonne National Laboratory (ANL) B Sandager, Peabody Museum of Archaeology and Ethnology, Harvard University SC Miller, WA Angus, University of Utah OG Raabe, University of California-Davis JC Prather, University of North Carolina RE Filipy, Washington State University-Tri-Cities SA Benjamin, Colorado State University JAL Dubeau, University of Southern California KL Jackson, University of Washington PR Watson, Oregon State University
High-Field ICR Mass Spectrometry of Large Molecules	RD Smith, SA Hofstadler, JE Bruce, AL Rockwood, PNL WS Hancock, Genentech JH Futrell, University of Delaware FW McLafferty, Cornell University
Ion Mobility Spectrometry Aerosol Technology Development	GA Eiceman, New Mexico State University AC James, JK Briant, BJ Greenspan, YF Su, MA Parkhurst, TE Hui, PNL R Akber, Alligator Rivers Region Research Institute, Northern Territory, Australia PK Hopke, Clarkson University YS Cheng, GJ Newton, ITRI SB Solomon, Australian Radiation Laboratory, Melbourne, Australia EO Knutson, AC George, KW Tu, Environmental Measurements Laboratory (EML) JP McLaughlin, University College, Dublin, Ireland JC Strong, AEA Technology, Harwell, England
Development of Radon Risk and Carcinogenesis Models	FT Cross, GE Dagle, RG Stevens, ES Gilbert, JA Mahaffey, AC James, RL Buschbom, PNL W Hofmann, University of Salzburg, Austria WB Lowrie, PJ Neafsey, University of Connecticut-Storrs SH Moolgavkar, Fred Hutchinson Cancer Research Center
Modeling Radon Lung and Organ Dose in Humans and Animals	AC James, TE Hui, KD Thrall, DR Fisher, FT Cross, AL Brooks, MR Sikov, HK Meznarich, GE Dagle, JK Briant, PNL NH Harley, BS Cohen, New York University Medical Center DL Swift, The Johns Hopkins University YS Cheng, RA Guilmette, ITRI A Birchall, NRPB, Chilton, England P Duport, Atomic Energy Control Board, Ottawa, Canada P Gehr, University of Bern, Switzerland R Masse, M Roy, Commissariat à l'Énergie Atomique (CEA), Fontenay-aux-Roses, France W Hofmann, University of Salzburg, Austria
In Vivo/In Vitro Radon Studies	FT Cross, AL Brooks, JK Briant, TE Hui, RF Jostes, JE Hulla, AC James, M Khan, LS McCoy, KD Thrall, PNL EW Fleck, Whitman College, Walla Walla, Washington L Lutze, University of California-San Francisco R Miller, E Hall, Columbia University RJ Albertini, JP O'Neill, University of Vermont SH Moolgavkar, Fred Hutchinson Cancer Research Center MR Raju, Los Alamos National Laboratory (LANL) HH Evans, Case Western Reserve University EJ Hall, Columbia University V Bond, Brookhaven National Laboratory (BNL) J Samet, New Mexico Tumor Registry



Table 4.2. (contd)

Genotoxicity of Inhaled Energy Effluents	AL Brooks, RF Jostes, M Khan, PNL R Kitchin, University of Wyoming, T Straume, JN Lucas, Lawrence Livermore National Laboratory (LLNL) WK Yang, Oak Ridge National Laboratory (ORNL) JM Tucker, LLNL
Tumor Suppressor Genes in Radiation-Induced Cancer	RP Schneider, PNL TM Seed, ANL
Inhaled Plutonium Carcinogenesis in Dogs	AL Brooks, JF Park, GE Dagle, RE Weller, CR Watson, ES Gilbert, PNL OG Raabe, University of California-Davis RL Perry, Michigan State University, E. Lansing, Michigan BB Boecker, ITRI B Carnes, Argonne National Laboratory SC Miller, University of Utah
Beagle Pathology Atlas	GE Dagle, PNL Pathologists at ITRI, ANL, University of Utah, Colorado State University, and University of California-Davis
Molecular Events During Tumor Initiation	DL Springer, BD Thrall, PNL R Novak, RC Zanger, Wayne State University, Detroit MJ Smerdon, DB Mann, Washington State University
Carbon Tetrachloride Health Risk	DL Springer, LB Sasser, JF Park, PNL RJ Bull, Washington State University
Application of Pharmacokinetics Analysis and Dosimetry to Species Difference in Sensitivity to Toxic Substances	DL Springer, EG Edmonds, SC Goheen, R Stenner, PNL RJ Bull, W Elmquist, DM Sylvester, Washington State University
Environmental Sciences Research Center	RE Wildung, PNL L Xun, Washington State University-Tri-Cities T Onstott, Princeton University K Di, Washington State University C Aguilar, Utah State University S Nierzwicki-Bauer, Rensselaer Polytechnic Institute D Boone, Oregon Graduate Institute D Balkwill, Florida State University G Pinder, University of Vermont PR Grossl, University of Delaware R Miller, Arizona State University
Arid Lands Studies	SO Link, H Bolton Jr., JL Downs, PNL JL Smith, JJ Halvorson, US Department of Agriculture, Agricultural Research Service at Washington State University, Pullman RA Black, DL Mummey, JL Healy, Washington State University
Multidimensional Modeling Describing Intermediate-Scale Flow Systems	EM Murphy, TR Ginn, BD Wood, YA Gorby, PNL J Cushman, Purdue University C Arola, University of Virginia NL Torres-Velázquez, University of Puerto Rico
Experimental & Modeling Studies of Organic-Radionuclide Interactions	JM Zachara, JP McKinley, JE Szecsody, SV Lee, SC Smith, PNL G Yeh, Pennsylvania State University John Westall, Oregon State University Laura Kuzel, Montana State University

**Table 4.2. (contd)**

Subsurface Organic Fluid Flow	RL Lenhard, CS Simmons, PNL D Rolston, University of California-Davis FAL Dullien, University of Waterloo
Microbial/Origins/Transport	EM Murphy, JA Schranke, PNL D Balkwill, Florida State University D Ringelberg, University of Tennessee
Improving the Biodegradative Capacity of Subsurface Bacteria	MF Romine, FJ Brockman, PNL R Reeves, D Balkwill, Florida State University
Subsurface Microbial Processes	JK Fredrickson, FJ Brockman, TO Stevens, PNL D Balkwill, Florida State University T Kieft, New Mexico Institute of Mining and Technology D Ringelberg, D White, University of Tennessee WM Huang, A Ferry, University of Utah D Stahl, N Fry, University of Illinois D Boone, Oregon Graduate Institute A Ogram, Washington State University
Biodegradative Enzyme Design	RL Ornstein, PNL SG Sligar, University of Illinois-Urbana DB Janssen, University of Groningen, The Netherlands LP Wackett, University of Minnesota-St. Paul JA Peterson, University of Texas Southwestern-Dallas
Nitrogen and Water Use Efficiency	SO Link, H Bolton Jr., JL Downs, PNL RA Black, Washington State University
Geosciences Testing	PE Long, SA Rawson, JK Fredrickson, JP McKinley, CJ Murray, CD Gullett, PL Gassman, BN Bjornstad, JM Zachara, PNL S Birnbaum, University of Texas-San Antonio D Balkwill, Florida State University T Kieft, New Mexico Institute of Mining and Technology TJ Phelps, ORNL FS Colwell, Idaho National Engineering Laboratory (INEL) T Griffin, BF Russell, Golder Associates TC Onstott, Princeton University AL Mills, G Hornberger, J Herman, University of Virginia
Protein Structure and Folding	RJ Douthart, PNL AK Dunker, R Miller, Washington State University
Medical Internal Dosimetry	DR Fisher, TE Hui, JS Durham, RL Hill, PNL ID Bernstein, F Appelbaum, D Matthews, Fred Hutchinson Cancer Research Center WB Nelp, JF Eary, OW Press, University of Washington Medical Center H Breitz, Virginia Mason Medical Center M Bjorn, NeoRx Corporation L Williams, J Wong, City of Hope Medical Center MW Geerlings, Pharmactinium, Arnhem, The Netherlands GV Dalrymple, D Colcher, University of Nebraska Medical Center EA Woltering, Louisiana State University JN Weinstein, National Cancer Institute S Larson, Memorial Sloan-Kettering Cancer Center MJ Swint, Hanford Environmental Health Foundation RL Kathren, Washington State University-Tri-Cities

Table 4.2. (contd)

Microdosimetry of Alpha and Beta Particles	DR Fisher, TE Hui, PNL EE Watson, M Stabin, Oak Ridge Associated Universities VP Bond, BNL
Capillary Electrophoresis	CG Edmonds, RD Smith, PNL H Yount, Washington State University D Liberato, Hoffman LaRoche AG Ewing, Pennsylvania State University
Advanced Mass Spectrometry	TN Davis, University of Washington CR Cremo, JNS Evans, JD Satterlee, MF Smerdon, R Yount, Washington State University MF Morales, University of the Pacific SG Sligar, University of Illinois DL and JD Smith, Purdue University CHL Schackleton, Children's Hospital Research Institute JK Barton, California Institute of Technology A Shephartz, Yale University C Hardin, North Carolina State University-Raleigh JH Futrell, University of Delaware FW McLafferty, Cornell University DJ Liberato, Hoffman-LaRoche, Inc. RN Riggan, Lilly Research Labs MM Siegel, Lederle Laboratories, American Cyanamid Company E Griffey, ISIS Pharmaceutical G Fong, Hybridon, Inc. W Hancock, Genentech, South San Francisco
Microdosimetry of Heavy Charged-Particle Beams	LA Braby, NF Metting, LH Toburen, PNL H Mensel, University of Saarlands, Hamburg
DNA Damage by Ionizing Radiation	LA Braby, JH Miller, AF Fuciarelli, PNL A Chatterjee, Lawrence Berkeley Laboratory (LBL) H Box, Roswell Park Memorial Institute C Swenberg, Armed Forces Radiobiology Research Institute J Raleigh, University of North Carolina EW Fleck, Whitman College, Walla Walla, Washington S Wallace, University of Vermont ME Schillaci, LANL C Benham, Mt. Sinai School of Medicine
Track Structure Applications	WE Wilson, JH Miller, PNL D Brenner, Columbia University D Goodhead, Medical Research Council, Harwell, England J Turner, R Richie, ORNL H Paretzke, GSF Neuherberg
Ionization in Ion-Molecule Collisions	RD DuBois, PNL ST Manson, Georgia State University H Schmidt-Böcking, KO Grueneveldt, University of Frankfurt R Olson, University of Missouri-Rolla ME Rudd, University of Nebraska C Drexler, University of Frankfurt/GSF Neuherberg D Schneider, LLNL
Biophysical Modeling	LA Braby, WE Wilson, JM Nelson, JH Miller, RL Ornstein, PNL R Rein, State University of New York-Buffalo S Curtis, LBL

Table 4.2. (contd)

	M Varma, DOE H Thames, MD Anderson Cancer Research Center M Zaider, Columbia University N Priest, Harwell, England R Kathren, Washington State University-Tri-Cities
Flow Cytometric Studies	JE Morris, JM Nelson, PNL HA Crissman, P Dean, LLNL S Smith-Carr, Tuskegee University
Multilab Collaboration on ASCOT Multi-Year Planning	CE Elderkin, JC Doran, CD Whiteman, DC Bader, PNL M Riches, DOE/ESD W Clements, LANL P Gudiksen, LLNL R Coulter, ANL WE Neff, NOAA/Wave Propagation Laboratory (WPL) R Hosker, NOAA/Atmospheric Turbulence and Diffusion Division (ATDD) R Addis, Savannah River Laboratory (SRL)
ASCOT Experimental and Modeling Research	DC Bader, X Bian, JC Doran, CD Whiteman, KJ Allwine, JM Hubbe, S. Zhong, PNL W Clements, J Bassert, JT Lee, LANL P Gudiksen, J Leone, R Lange, LLNL R Coulter, ANL C Nappo, NOAA/ATDD R Banta, NOAA/WPL J Riley, University of Washington
Atmospheric Chemistry Program	CM Berkowitz, KM Busness, RG Chapman, MT Dana, RC Easter, R Saylor, WGN Slinn, S Smyth, PNL P Daum, L Kleinman, BNL JM Hales, ENVAIR C Spicer, Battelle Columbus Division M Wesley, ANL R Charlson, University of Washington L Peters, University of Kentucky
Electrospray Ionization Mass Spectrometry	RD Smith, JA Loo, HR Udseth, KJ Light-Wahl, RR Ogorzalek Loo, BE Winger, PNL C Shackleton, University of California-San Francisco
High-Field NMR Research	TS Tenforde, PD Ellis, GP Drobny, MA Kennedy, PNL BR Reid, University of Washington AK Dunker, JD Satterlee, JNS Evans, Washington State University H Box, Roswell Park Memorial Institute
Circular Dichroism Effects in Multiphoton Ionization Processes	RJ Miller, JE Murphy, RG Tonkyn, PNL RN Compton, ORNL V McKoy, California Institute of Technology, Pasadena
<i>Ab Initio</i> Theories of Excited State Properties	RJ Miller, PNL DF Feller, ED Glendening, PNL

Table 4.2. (contd)

<b>ARM Program:</b> Management Team	E Baroni, TS Cress, J Griffin, G Rudy, W Pennell, W Spaeth, G Stokes, PNL S Barr, LANL M Dickerson, LLNL P Lunn, A Patrinos, P Crowley, DOE D Renne, National Renewable Energy Laboratory (NREL) S Schwartz, BNL J Vitko, SNL P Singhey, ORNL ML Wesely, ANL
Science Team	JC Doran, SJ Ghan, CD Whiteman, PNL T Ackerman, G Young, Pennsylvania State University F Baer, R Ellingson, University of Maryland J Kao, LANL J Morcrette, European Center for Medium Range Weather Forecast, England G Holland, Bureau of Meteorology Research Center, Australia RN Byrne, Science Applications International Corporation L Harrison, JJ Michalsky, CJ Walcek, Wei-Chyung Wang, State University of New York-Albany R Cess, P Varanasi, State University of New York-Stonybrook S Clough, J-F Louis, Atmospheric and Environmental Research, Inc. P Davis, L Stowe, NOAA/National Environmental Satellite Data and Information Service W Cotton, P Gabriel, D Randall, G Stephens, W Gray, Colorado State University R Coulter, ANL J Curry, P Webster, University of Colorado W Dabberdt, D Parsons, Atmospheric Technology Division H Revercomb, University of Wisconsin, Madison K Gage, R Kropfli, ER Westwater, W Eberhard, C Grund, NOAA/ERL C Gautier, University of California-Santa Barbara A Heymsfield, J Kiehl, D Parsons, NCAR M Bradley, J Penner, LLNL AA Lacis, J Spinhirne, W Wiscombe, A DelGenio, H Melfi, NASA/Goddard Space Flight Center PJ Lamb, University of Oklahoma R McIntosh, University of Massachusetts J Hudson, D Mitchell, Desert Research Institute D Murcay, University of Denver CMR Platt, Commonwealth Scientific and Industrial Research Organization (CSIRO), Division of Atmospheric Research, Australia S Raman, North Carolina State University V Ramanathan, University of California-San Diego K Sassen, S Krueger, University of Utah WL Smith, RB Stull, University of Wisconsin R Somerville, Scripps Institute of Oceanography K Stamnes, University of Alaska O Toon, NASA D Westphal, Ames Research Center VE Zuev, Institute of Atmospheric Optics, Russia
Site Managers	B Clements, LANL DL Sisterson, ANL B Zak, SNL
Site Scientists	T Ackerman, Pennsylvania State University PJ Lamb, University of Oklahoma K Stamnes, University of Alaska

**Table 4.2. (contd)**

North Atlantic Regional Experiment	CM Berkowitz, KM Busness, RD Saylor, PNL P Daum, L Kleinman, BNL J Weinstein-Lloyd, State University of New York-Old Westburg F Fehsenfeld, W Parrish, NOAA/Environmental Research Laboratory G Issac, AES-Canada JM Hales, ENVAIR
Mechanism or Radon Induced DNA Damage	L Lutze, J Cleaver, UCSF JP O'Neill, R Albertini, University of Vermont
Correlation of DNA Single-Strand Breaks	W Morgan, UCSF
Modeling Cellular Responses to Genetic Damage	A Chatterjee, Lawrence Berkeley Laboratory
Perturbations of DNA Structure and Dynamics	B Hingerty, Oak Ridge National Laboratory R Osman, Mount Sinai School of Medicine
<b>Subsurface Science Program/ESRC</b>	
Microbial Ecology/Deep Microbiology	D Balkwill, Florida State University
Anaerobic Bacteria/Deep Microbiology	E Stevens, Memphis State University
Multiphase Fluid Dynamics/Multiphase Fluid Flow	L Prunty, North Dakota State University
Anaerobic Microbiology/Deep Microbiology	D Boone, Oregon Graduate Institute
Fluid Inclusions and Microbial Origins/Deep Microbiology	TC Onstott, Princeton University
Interphase Mass Transfer/Multiphase Fluid Flow	G Pinder, Princeton University (through 1990)
Hydrogeology, Applied Mathematics/Microbial Origins, Natural Heterogeneity	T Ginn, Purdue University
Molecular Biology/Deep Microbiology	S Nierzwicki-Bauer, Rennselaer Polytechnic Institute
Multiphase Transport/Multiphase Fluid Flow	R Miller, University of Arizona
Microbial Intrinsic Resistance to Metal/Deep Microbiology	A Summers, University of Georgia
Site-Directed Mutagenesis/ESRC Remedial Concepts	S Sligar, University of Illinois

**Table 4.2. (contd)**

Microbial Adhesion and Microbial Origins/Deep Microbiology	M Fletcher, University of Maryland
Fluid Flow and Transport/Coupled Processes	S Silliman, University of Notre Dame
Anaerobic Microbiology/Deep Microbiology	T Phelps, University of Tennessee
Integrated Subsurface Modeling/Multiphase Fluid Flow	G Pinder, University of Vermont
Clay Mineralogy and Iron Speciation	R Ferrell, Louisiana State University
Anaerobic Microbial Analysis	J Suflita, University of Oklahoma
Microbial Origins	W Huang, University of Utah

**Table 4.3. License Agreements and Patents**

Patent No.	Technology	Inventor(s)	Effective Date
B-0909 CIP2	Detection and Differentiation of <i>Coxiella burnetii</i> In Biological Fluids (Q-Fever)	ME Frazier, JE Samuel, OG Baca, LP Mallavia	11/02/93
B-1247	Method for Increase Sensitivity of Radiation Detection and Measurement	SD Miller	10/11/94
E-0670 CIPR	Combined Electrophoresis-Electrospray Interface and Method	RD Smith, HR Udseth, JA Olivares	10/18/94
E-0863 CIP	Method for Radiation Detection and Measurement	SD Miller	12/21/93
E-0939	Apparatus for In Situ Calibration of Instruments that Measure Fluid Depth	MD Campbell	01/11/94
E-0976	Enhancement of In Situ Microbial Remediation of Aquifers	JK Fredrickson, FJ Brockman, GP Streile, JW Cary, JF McBride	11/30/93
E-1063	Fractional Channel Multichannel Analyzer	LE Brackenbush, GA Anderson	08/23/94
E-1090	An Improved Combined Electrophoresis-Electrospray Interface and Method	CJ Barinaga, HR Udseth, RD Smith	06/13/95
E-1115	Prehensile Apparatus (Robotic Finger)	CM Smith	10/12/93
E-1156	Lung Pair Phantom	PC Olsen, NR Gordon, KL Simmons	11/30/93

**CRADAs Related to OHER-Sponsored Research at PNL**

Principal Investigator	Industry Participants	Project Title
PA Eschbach	Instrumentation Northwest	HydroProbe Technology
RA Bair	Kendall Square Research Corporation	Software for High Performance Computing
LJ Kangas	Cadwell Laboratories, Inc.	Artificial Neural Networks to Assess Adequacy of Anesthesia
AA Campbell	Health Tech Development, Inc.	Bioactive & Porous Metal Coatings for Improved Tissue Regeneration
BW Wright	E.I. DuPont De Nemours & Company	Supercritical Fluid Extraction Instrumentation for Pesticide Residue Analysis

**Licenses**

Effective Date and License No.	Type of Agreement	Technology
05/15/94 93224-C	Nonexclusive, Worldwide Patent & Technical Information license	Liquid Monitoring Sensor
12/06/94 94297-C	Exclusive Patent License	Electronic Dendrometer
12/01/94 94151-C	Exclusive Worldwide License	Software: NUCLIDES Database Mgmt Tool for the Erdtmann-Soyka Library
10/20/94 94236-O-C	Option to an Exclusive Worldwide Patent & Technical Information License	Void Metal Composite and Surface Mineralization
10/15/93 93112-C	Worldwide, Nonexclusive Patent & Technical Information License	Submersible Ion-Selective Electrode w/Improved Capillary Design
03/15/95 95006-C	Nonexclusive License	Software: MMED/Multimedia-Modeling Environmental Database
06/09/94 9130-C	Exclusive, Worldwide License	Cooled, Optical Luminescence Dosimetry (COLD) and Optical Luminescence Dosimetry (OLD) Technology
12/25/94 94329-C	Nonexclusive, Worldwide License	Software: SYNTH/Program for Generating Synthetic Gamma Ray Spectra
12/28/94 94331-C	Nonexclusive, Worldwide License	Software: MMED/Multimedia-Modeling Environmental Database



**Table 4.4. Examples of Work for Other Department of Energy Components and 1830-Related Services**

Related to OHER Budget Category	Sponsor	Project Title	Principal Investigator	FY 1995 Budget (\$K)
KP-01	BES	Supercritical Fluid Studies	Fulton	430
KP-01	BES	Laser Spectrometry	Miller	75
KP-01	BES	Analyze Mass Spectrometry Research	Gordon	450
KP-02	EPA	Comprehensive Model Evaluation	Barchet	50
KP-02	DOD	BRL Range 14 Air Clean	Glissmeyer	40
KP-02	DOE/Fossil Energy	Visibility Assessment	Laulainen	100
KP-02	NRC	Emergency Response Support	Ramsdell	86
KP-02	USDA/USFS	Spray Drift Model	Whiteman	16
KP-02	EPA	Contaminant Transport	Criscenti	96
KP-02	DOD	Cell Bioremediation	Truex	193
KP-02	NRC	Characterization of Radionuclides	Serne	299
KP-02	EPA	Geochemical Modeling	Jenne	908
KP-02	DOD	Smoke and Obscurants	Sehmel	400
KP-02	EPRI	Regional AQ Model Evaluation	Barchet	10
KP-02	USFS	Topographic Shading	Whiteman	3
KP-02	DG&E	Emergency Response Application	Allwine	3
KP-02	EPA	Comprehensive Model Evaluation	Barchet	75
KP-02	DOD	Endangered Threatened Species	Brandt	400
KP-02	DOD	Vegetative of Yakima Firing Center	Cadwell	800
KP-03	EH-42/NIOSH	Hanford Health and Mortality Study	Gilbert	141
KP-03	EH-42	Iron Stores and Risk of Cancer	Stevens	68
KP-03	NCI	Exposure in Radon Epidemiology	Mahaffey	97
KP-03	BPA	Cancer Increase Study Methodology	Sever	31
KP-03	NRC	Fetal Dose from Radionuclides	Sikov	113
KP-03	DOE	Biological Effects of Electromagnetic Fields	Anderson	787
KP-03	NASA	Space Dosimetry	Braby	560
KP-05	EPA	EMAP Environmental Information	Thomas	600
KP-05	EPA	Global Change Study System	Barchet	190
KP-05	EPA	Integrated Climate Change Analysis	Edmonds	500
KP-05	NASA	Radiative Impact of Aerosols	Ghan	160
KP-06	NCI	Therapy of Leukemia and Lymphoma with Monoclonal Antibodies (joint project with Fred Hutchinson, Cancer Research Center, Seattle, Washington)	Fisher	25

## **5.0 Program Orientation and Future Directions**

The projected evolution of OHER programs for the period FY 1995-1997 is discussed in this section of the report. Facility construction and modifications to support research are listed in Table 5.1. Table 5.2 lists examples of major equipment requirements for the 3-year period.

### **5.1 Analytical Technology (KP-01)**

As noted in Section 4, this area of research is in transition. Two projects associated with the measurement science portion are being wound down. The mass spectrometry research that was funded under this activity is retooling and will be involved with future health effects research efforts.

### **5.2 Environmental Research (KP-02)**

#### **5.2.1 Atmospheric Science (KP-02-01)**

Atmospheric research at PNL addresses the local-, regional-, and transcontinental-scale effects of the emissions of energy-related pollutants on air quality and deposition that are critical to the implementation of the Energy Policy Act of 1992. Research on surface energy exchanges over inhomogeneous surfaces and the interactions of thermally-driven circulations induced by local terrain features with larger scale flows established the transport and dispersion of pollutants in the atmospheric boundary layer. Research on atmospheric homogenous and heterogenous chemical reactions involving energy-related and natural emissions and the processing of emissions and reaction products by clouds is directed to understanding the fate of those pollutants. Beginning in FY 1995, these research thrusts will be ever more closely coupled to better respond to the needs of OHER.

The focal point for that coupling is the need for an improved understanding of the interaction between the diurnally evolving chemical and physical structures of boundary layer. The interaction of the surface mixing layer and the overlying free troposphere on the atmospheric chemistry of the mixing layer is recognized as an area of research vital to the North American Research Strategy on Tropospheric Ozone.

PNL will bring several important capabilities to bear on this research area:

- the Gulfstream 1 (G-1) research aircraft, which PNL operates for OHER as the DOE Aircraft Research Facility
- radar and sodar profilers and laser anemometers, which provide remote sensing of the dynamical and thermal structure of the boundary layer

- a coupled mesoscale meteorological and chemical transport modeling system, which is based on the Colorado State University Regional Atmospheric Modeling System (RAMS) and PNL's Global Chemistry Model (GChM).
- a cluster of four high-performance IBM/RISC 6000 scientific work stations, which are interconnected for coarse-grained parallel as well as sequential computation.

These capabilities will be used in an integrated program of field studies, data analysis and interpretation, and numerical modeling that focuses on the daily cycling of the chemical, thermal, and dynamical structure of the boundary layer and lower troposphere. Research projects with DOE's Atmospheric Chemistry Program (ACP) and the Atmospheric Studies in Complex Terrain (ASCOT) program support this work.

The G-1 Research Aircraft Facility is a vital component of the Atmospheric Chemistry Program's research agenda. Continual investment into state-of-the-art instrumentation is required for this facility to meet the needs of its users. The general requirements for new instrumentation include 1) better limits of detection and sensitivity, 2) faster response to changes in the measured quantity, or 3) the capability for measuring new chemical compounds or physical parameters in the atmosphere.

### **5.2.2 Terrestrial Transport (KP-02-03) and Ecosystem Functioning and Response (KP-02-04)**

This research is focused on developing a fundamental understanding of key processes controlling chemical behavior and biological processes in subsurface and terrestrial systems. Coupled with advanced sampling methods and statistical scaling studies, these efforts form the basis for examination of the response and recovery of subsurface systems in environmental restoration, particularly bioremediation, and for early detection of global changes. The research integrates technical strengths in biogeochemistry, environmental microbiology, molecular biology, plant physiology, hydrodynamics, and theoretical ecology. Research on the mechanisms of molecular interactions at environmental interfaces and on elucidation of the enzymatic basis for key biological processes uses analytical tools from the molecular sciences. As part of PNL's ESRC and the Global Environmental Change (GEC) initiative, advanced scaling methods are used in conjunction with field experimentation and observations to extrapolate process-level understanding to the pathway and system levels. Premier research facilities (subsurface environmental research facility, arid land watershed facility), as well as the Environmental Research Park and deep subsurface exploration and field observations at DOE sites, play vital roles in this multitiered research approach in which laboratory, intermediate-scale, and field studies are conducted interactively to resolve key questions. The intermediate-scale facilities allow measurements of the effects of multiple phenomena under controlled conditions. Field studies aid in parameterization of laboratory and intermediate-scale research, and in validating concepts and models at both the local and regional levels. Strong university relationships are being expanded to form consortia for efficient use of PNL laboratory and field facilities. The PNL ESRC plays a key role in transferring the results of scientific research to other DOE components, other federal agencies, and industry for improving the environment and for developing new industrial processes and products.

Chemical, microbial, hydrologic, and plant processes interact in complex ways that must be resolved before accurate predictions can be made of human exposure to inorganic and organic contaminants from energy- and defense-related activities. PNL has pioneered research on the terrestrial and subsurface geochemical and biological interactions that control the chemical form and behavior of chemical species in terrestrial and groundwater systems. Current research emphasis is on subsurface phenomena controlling the behavior of inorganic cations (organic complexation) and anions (oxidation, reduction), and of organic contaminants (multiphase flow). The latter effort is maturing and engaged actively in technology transfer through "hands on" workshops at DOE sites. In addition to helping establish a sound basis for developing and calibrating the next generation of contaminant and bacterial transport models, this effort is making major contributions to our general understanding of fluid dynamics and elemental cycling in the environment. This research in conjunction with other efforts in bacterial transport also provides a unique basis for using natural processes such as in bioremediation for restoration of contaminated environments, a long-range objective of the ESRC. The PNL programs are focusing on the fate of contaminants mobilized from DOE mixed wastes (e.g., radionuclide and organic complexes) and the role of deep subsurface microbial populations in diverse heterogeneous hydrogeologic environments characteristic of DOE and other waste sites nationwide.

A new Laboratory initiative in microbial biotechnology is building, in part, on the SSP's deep exploration efforts, adding new dimensions in environmental microbiology, genome sciences, bioremediation, and bioprocess engineering. LDRD investments are building new capabilities in these areas, laying the groundwork for a broad-based program in biotechnology over the next 5 to 10 years.

The majority of environmental impacts from land extraction of energy resources will continue to occur in arid and semiarid regions. These impacts may fundamentally alter processes important to ecosystem and global functioning. The ALE Reserve provides a unique opportunity to identify and quantify the processes associated with these impacts. Field experiments on the ALE Reserve are using altitudinal gradients and systematic alteration of water and nutrient dynamics to simulate climate changes and define important interactions among representative biological, hydrologic, and biogeochemical processes. Specialized techniques and equipment (e.g., radiotracers, weighing lysimeters, rainfall simulations, and instrumented watersheds) allow evaluations of the controls on critical processes that govern the ecosystem's response to and recovery from stress. Advanced designs for ecosystem experiments, scaling methods, and models are under development to determine impacts and extrapolate results to regional and global scales. Further efforts will be directed toward closer interaction with other DOE sites to compare and evaluate long-term databases for use in understanding the impacts of energy development at the landscape level.

## **5.3 Health Effects (KP-03)**

### **5.3.1 Biological Research (KP-03-02)**

Biological research is addressed through a multilevel approach incorporating studies from the molecular to whole-animal levels. Emphasis is placed on gaining a quantitative understanding of dose-effect relationships and mechanisms that underlie the effects of radiation and chemicals using integrated dosimetric, molecular, genetic, cellular, and experimental animal approaches. Our program includes

basic studies to test hypotheses concerning the interaction of chemical and physical agents with molecules in biological systems, and the alteration of these molecules by the transfer of energy. Alterations of the structure and function of genetic processes are investigated both in vivo and in vitro as biological indications of the development of subsequent disease processes in living animals. The ultimate objective is to identify the cause of, and to predict human susceptibility to, disease states induced by exposure to radiation or toxic chemicals.

In FY 1994 and FY 1995, dose-effect relationship studies of inhaled plutonium in rats are being completed. Studies of inhaled plutonium in dogs will also be completed by FY 1996.

Biological research at PNL will begin to stress

- molecular and structural biology studies of DNA damage and repair
- high-LET radiation damage using PNL's unique resources
- genetic susceptibility.

**Molecular Structure/Function Studies.** Structural biology will continue to grow at PNL from FY 1995-1997. A Basic Life Sciences initiative, funded through LDRD, has led to the integration of molecular biology with advanced experimental techniques, such as NMR and MS for analyzing molecular structures, and the advanced computational and modeling capabilities in the EMSL.

The EMSL computational resources will allow PNL's Health Effects Program to apply new theoretical and computational approaches to understanding mechanisms involved in mutagenesis, carcinogenesis, and developmental abnormalities through modeling three-dimensional structures of macromolecules. The EMSL also provides advanced spectroscopic techniques for structural biology investigations relevant to molecular biology research. For example, three-dimensional information on chromatin/nucleosome structures will complement laboratory studies on the influence of bulky adducts on gene expression.

PNL's program in the molecular and structural biology of DNA damage and repair will include studies of recognition of DNA damage by proteins. This is a critical issue in genome protection and will take full advantage of the EMSL resources and the key molecular biology skills at PNL. Of particular interest is the influence of DNA damage on the recognition of specific DNA sequences by proteins such as transcription factors and the general properties of damaged DNA that signal the binding of damage recognition proteins.

While key proteins have been identified for recognizing and repairing several types of DNA damage, the proteins required for the recognition and repair of cyclic nucleotide damage have not been described. This type of damage represents a common event from ionizing radiation, yet the biological consequences are unknown. New research at PNL will begin to describe the influence of this type of damage on cellular processes including replication and transcription and the mechanisms for its repair.

In cells, DNA damage recognition takes place within the context of chromatin. Thus, studies are also planned to determine how nucleosome structure influences DNA damage recognition. This work will benefit from the continuing research on chromatin's role in damage repair, particularly with respect to transcriptional activity of the gene.

Following recognition of DNA damage, cell signalling pathways are responsible for recruiting additional DNA repair proteins and for directing the alternative consequences for the cell. For example, apoptosis or cell cycle arrest can result from DNA damage recognition. The mechanisms responsible will be the focus of new studies in this area.

**Effects of High-LET Radiation.** In vitro studies incorporating molecular and cellular biology and dosimetry to understand the molecular mechanisms leading to radiation damage at the cell level will be taking increasing advantage of PNL's unique resources for exposing cells to high-LET radiation. The microbeam irradiator is capable of targeting individual cells with single or multiple particles of defined energy. In addition, PNL has unique capabilities for exposing cells in culture to radon.

Cellular level research concerning cellular effects from high-LET radiation will continue to focus on markers of DNA damage, but with an increasing emphasis on a molecular level understanding of the events. Cell cycle regulation and the involvement of specific photo-oncogenes will be a major thrust.

**Genetic Susceptibility.** In the next 3-year period, research on genetic susceptibility will continue to become a focus of PNL's biological effects program. The recently initiated study on genetic susceptibility to radon-induced lung cancer has provided an exceptional model for identifying, mapping, and eventually cloning the genes responsible. Research has shown that two strains of mice, A/J and C57BL/6J, differ markedly in their susceptibility to radon-induced lung tumors. Successful identification of the contributing genes will provide tools for identifying individuals at risk and for understanding the fundamental mechanisms for those tumors.

Additional genetic susceptibility research is being applied to the issues of DNA damage and repair. These studies will complement ongoing programs in DNA repair and couple with the newer directions in molecular and structural biology.

**New Developments.** We are excited about two new developments in our future biological research programs. The first involves a novel strategy regarding health effects research; that is, coupling our unique EMSL instrumentation and capabilities in structural biology with grand challenge questions dealing with the correlation of structure and function. Second, within the EMSL we have developed a near field optical microscope (NFOM) which is ideally suited for investigating biological systems. The importance of the NFOM is that it surpasses the "diffraction limit" which is not being able to resolve features that are smaller than the wavelength of light used in the microscope. Following is a brief description of both of these approaches.

Perhaps the greatest challenge of our time is the correlation between structure and function in biological systems. The particular focus of our future health effects program is the structural and dynamic basis for the recognition and repair of damaged DNA and the cellular consequences to this

damage if it is not repaired. Cells can respond to DNA damage through a myriad of mechanisms with a common goal of protecting the whole organism. The loss of control at the cellular and tissue levels is a phenomenon common to all cancers and many developmental disorders. Underlying this are both transient and permanent alterations in the control of gene expression. Therefore, an understanding of the mechanisms by which cells control the expression of the genome after DNA damage is an important common denominator in our pursuit to understand the basis for health effects.

The disciplines of molecular and structural biology become entwined in the study of the cellular responses to DNA damage. The mechanism by which DNA repair enzymes recognize the presence of damage is unclear, as are the mechanisms by which damage recognition and repair triggers alterations in gene expression. Clearly, protein-DNA and protein-protein interactions control pathways which define the response of a particular cell to DNA damage. Such interactions are not limited to that of the repair proteins with damaged DNA but also include transcription factors which function to regulate the expression of gene products and thereby also protect the higher-order integrity of the organism. In addition, the structure of the chromatin itself needs to be determined since it is becoming clear that histone-DNA interactions are not static and contribute to the control of gene expression. Protein-protein interactions involved in the signaling of DNA damage must also be examined since it is these pathways which bridge the recognition of DNA damage with changes in gene expression. Therefore, at all levels, the control of gene expression also becomes both a molecular and structural question, and an understanding of this process requires an integrated effort from both disciplines. Finally, molecular and structural studies must be integrated with an understanding of the pathology at the cellular, tissue, and whole organism levels in order to achieve the final goal of understanding regulation of the human genome and its consequence to human health.

We have developed a NFOM which enables the study of individual molecules and aggregates in specific physical environments. There are two major laboratories developing this type of instrument: PNL and Bell Labs. The heart of the NFOM is an optical fiber pulled and coated, leaving a sharp tip with an approximately 20-nm opening, roughly the size of a single protein molecule. The fiber is mounted as a replacement for the tip in an atomic force microscope (AFM) and operated as an AFM to obtain a topographic image of the sample. Simultaneously, the sample is excited with light emanating from the fiber tip and the induced fluorescence is detected and analyzed to obtain an optical image of the sample of specific molecules on the surface at 5 to 10 times the resolution obtained with the best existing optical microscopes. In this manner we have obtained, for the first time, topographical images and fluorescence lifetimes of a single protein complex; the light harvesting complex in an intact photosynthetic membrane. The NFOM has been modified for "under water" operation to allow in situ characterization of biological systems. Applications range from biological, to environmental, to materials science. The development of this instrumentation is being supported by OER/BES research and Cooperative Research and Development Agreement (CRADA) funding. Novel applications of the NFOM are being developed for various OHER programs, e.g., structural biology applications applied to problems in bioremediation.

### 5.3.2 Radiological and Chemical Physics (KP-03-03)

An understanding of the RBE of high-LET radiation, including dose and dose-rate effects, rests on our ability to understand the fundamental physical, chemical, and biological processes initiated by the

absorption of energy from a radiation field. This program will continue to encompass an integrated multidisciplinary effort to better understand those processes at the cellular and molecular levels. Experimental studies are conducted in radiation physics and chemistry to provide input data to models of radiation action in macromolecular systems such as DNA plasmids. These studies, in turn, will provide guidance and tests of evolving mathematical models. Increased emphasis will be directed toward understanding the effects of molecular structure and environment on energy deposition and energy transport. New studies of electron transport in condensed-phase material, including DNA, are in progress. Theoretical studies address the influence of chromatin structure on radiation-induced alterations in DNA, with special attention given to correlations between the spatial pattern of energy deposition and the structure of the macromolecular target. Biophysical models are being developed that incorporate greater detail regarding the molecular characteristics of the cellular system. Work in these areas will be tightly coupled to research in the areas described above.

## **5.4 General Life Sciences (KP-04)**

### **5.4.1 Structural Biology (KP-04-02)**

Rational enzyme redesign is a coupled experiment-theory approach designed to 1) provide a fundamental understanding of enzyme structure-function-dynamic relations, in biotic and extreme environments, and 2) achieve planned enzyme alternate-use objectives, in a timely manner. Developing a rational enzyme redesign capability is, without doubt, of immense proportion in view of increasing environmental concerns, regulatory constraints, limitations in natural resources, and dependency on foreign fossil fuels. Rational enzyme redesign is currently under way in two areas: 1) improving specificity and kinetics of enzyme-mediated biodehalogenation, and 2) expanding the physical and chemical functional range of enzymes. Successful rational enzyme redesign will lead to improved subsurface in situ bioremediation of mixed wastes and many potential derivative biotechnological impacts. Rational enzyme redesign is and will take advantage of the explosive rate of new protein structures being deposited in the Brookhaven Protein Data Base, about 100 per month. Rational enzyme redesign will play an increasingly important role as computational power and modeling and simulation software continue to evolve.

### **5.4.2 Genome (KP-04-04)**

A research project that supports the OHER Human Genome Program is developing a computer graphics interface to the vast amounts of DNA sequence and physical mapping information that is being generated. The GnomeView software, which graphically represents information from the chromosomal level to the actual DNA sequence level, is currently in a beta-testing phase at 19 sites around the world. Color graphics images of database information provide a global view that yields information about the nature of the human genome. Local abstractions of GenBank (DNA sequence) and Genome Data Base (GDB) are accessed by query and mapped to pictorial representations of chromosomes and sequence. GnomeView presents a seamless integrated transition between these two databases. Run time access to the OMIM (Online Mammalian Inheritance in Man) database is available, providing detailed descriptions of various genome loci. Initial feedback on the GnomeView software has been encouraging, and a GnomeView user community is developing.



The program to develop ICR-MS techniques for rapid DNA sequencing will focus on improving the methods for ionization of large DNA segments used as starting material. Investigations will be carried out on the gas-phase processes necessary to obtain DNA sequence data by a stepwise degradation of the biopolymer. Proof-of-principle experiments on DNA sequencing efficiency will be performed with the new 7-tesla ICR-MS system.

In another component of the program to develop automated DNA sequencing technology, preliminary proof-of-principle experiments have been completed with a rotating drum electrophoresis apparatus, and the results have led to new design criteria for the apparatus that will make it even more efficient. Experiments are currently being conducted with a modified prototype apparatus.

## 5.5 Global Change Research Program (KP-05)

PNL's global change research program will continue its emphasis on

- improving the basic understanding of the physical, biological, and social sciences related to global environmental change
- understanding the role of economic development and technology both as a cause of, and a remedy for, global environmental change
- informing government policy relative to the energy, environmental, economic development, and national security aspects of global environmental change.

We will continue to place emphasis on the development of modeling tools that integrate our knowledge of the physical, biological, and socio-economic processes that form the complex problem of global environmental change. These tools will allow us to understand the impacts of changes in the physical environment on biological systems, economic resources, and human systems, and to determine the impacts that changes in these systems might have on the physical environment. At the same time, we will continue to conduct basic research on atmospheric and oceanographic processes important to the problem of global climate change, and we will increase research into the problem of regional climate change and its effects on water resources, agricultural productivity, and unmanaged ecosystems. Finally, we will build on the knowledge gained through our state-of-the-art assessment of social sciences and global environmental change to develop new research initiatives in this important area.

We will continue to be substantially involved in management of the Atmospheric Radiation Measurement Program and in the research carried out under this program. Development of the Southern Great Plains ARM site will be completed as deployment of ARM instrumentation in the Tropical Western Pacific and the North Slope of Alaska gathers momentum. The focus of activities will increasingly shift to continuous improvement in the data supplied to the ARM Science Team and in the design and execution of ARM experiments.

In PNL's ARM Science Team research projects, work will continue on the development of a stratiform cloud parameterization scheme for global climate models, research on the climatic effects of

mesoscale phenomena in the southern Great Plains, research to improve the representation of heterogeneous surface exchange processes in climate models, and the development and testing of a boundary layer radiometric profiler.

Energy emissions research will continue to improve the reliability of forecasting emissions of CO<sub>2</sub> and other radiatively active gases by developing a Second Generation Model (SGM) advanced emissions model. Model development, validation, and uncertainty evaluations depend on improved and expanded databases, including more definitive information on energy production and consumption practices, particularly for non-Organization for Economic Cooperation and Development (non-OECD) countries. Both China and the Former Soviet Union are major sources, and consumers, of energy supplies for which data must be organized by sector (residential, commercial, transportation, industrial, and agricultural). Model improvements and database development will be the primary emphasis in this research during the next few years. The program will focus on the implementation of improved versions of the SGM; and on the continued development of international modules, including the completion of modules for Korea, Japan, Canada, Mexico, and Western Europe. We expect to see increasing emphasis on the development of a family of integrated assessment models based on the SGM. These models will assimilate current understanding of the interactions between global energy generation and use, economic activity, climatic change, and the response and feedbacks from managed (i.e., agriculture) and unmanaged ecosystems. PNL is an international leader in this research. We expect these models to provide new insights into the complex interactions between human activities and the environment, and we anticipate that they will find increasing applications in the area of policy assessment.

Ocean research related to CO<sub>2</sub> and climate change will continue to focus on improving our understanding and ability to model key ocean mixing and interfacial transport processes, and on improving measurement technology for oceanographic research. The program will conduct experimental, theoretical, and modeling studies of exchange processes at the air-sea interface, and will conduct modeling experiments to improve the understanding of, and the parameterization in, large-scale models of the processes that govern the exchange of heat, mass, and momentum between the ocean's mixed layer and deeper regions. Understanding these processes is key to improving our ability to predict energy and gas transfers to the ocean and to clarifying the role of the oceans in controlling climate change. Physical, chemical, and biological processes involved in transfer mechanisms at the sea surface, such as bubble plumes and surface microlayer films, will continue to be studied experimentally to reduce uncertainties in predictions of transfer rates. Research in ocean dynamics will emphasize understanding of the processes that govern mixing across the thermocline and control the formation of deep water. Ocean dynamics studies will focus on the effects of Langmuir circulation on surface-layer mixing and upper ocean structure in the equatorial Pacific. Additional experiments will be completed to delineate the climatic factors that influence deep convection and deep water formation. In our CHAMMP project, we will be evaluating and improving the performance of the deep convection parameterization scheme in OGCMs.

## 5.6 Medical Applications (KP-06)

Through a Medical Systems and Technology initiative, PNL is actively developing new programs in the areas of medical imaging utilizing nonionizing radiation modalities, sensor technology for on-line radiation dosimetry and noninvasive physiological monitoring, application of powerful computational techniques for telemedical networking and the analysis of large data sets, production of new biocompatible materials for prosthetic devices and bone grafting, and synthesis of new classes of radiolabeled immunoconjugates that incorporate alpha-emitting radionuclides for tumor therapy. In the last of these areas, the new classes of densely-ionizing alpha emitters that are being produced and tested in collaboration with several universities and medical centers include bismuth-213, radium-223, and actinium-225. Research is being conducted on the complexation and linking of these radionuclides to monoclonal antibodies used as tumor-targeting vehicles. Immunoconjugate development will be followed by biodistribution and toxicity studies in laboratory animals. If the results of these initial studies are favorable, efficacy studies will be conducted with human tumors xenografted into immunodeficient mice and treated with alpha-emitting radiolabeled antibodies.

## 5.7 Environmental Molecular Sciences Laboratory

The Environmental Molecular Sciences Laboratory (EMSL) was first proposed as a major PNL initiative in FY 1989 and was carried forward as an initiative through FY 1992 at which time it received funding from DOE. The EMSL is a key component in PNL's effort to continuously develop and maintain the fundamental science base necessary to support DOE's strategic objectives. The objective of EMSL research is to advance the fundamental knowledge of the molecular sciences and to apply the knowledge gained from these advancements to environmental quality and fundamental science and technology issues of importance to DOE. The EMSL will be a first-of-a-kind collaborative research facility dedicated to advancing the molecular sciences.

Construction of the new 200,000 ft<sup>2</sup> laboratory began in the fourth quarter of FY 1994; the facility is scheduled to begin full operation early in FY 1998. The EMSL will contain laboratories, offices, computer and graphics rooms, shops, a library, and a seminar area including an auditorium. The laboratories will be arranged in topical clusters, including facilities for nonlinear optics and chemical kinetics research, interfacial structure analysis, aerosol research, chemical synthesis, sensor research, biomolecular structure analysis, and analytical chemistry. These laboratories will feature specialized equipment that includes an ultrafast laser spectroscopy unit (100 femtosec); high-field, two-dimensional NMR spectrometers (500, 750, and 900-1000 MHz) for studies on solids and liquids; laser Raman, Auger electron, x-ray photoelectron, and Fourier transform infrared spectrometers; mass spectrometers with ancillary molecular separation techniques; a scanning tunneling microscope; an atomic force microscope; a near field optical microscope, and x-ray diffraction instruments.

Although the EMSL will not be fully operational until FY 1998, some of its capabilities are being developed in interim facilities at PNL and are available for research that can be phased in between now and FY 1998. In addition, the EMSL research organization is being developed and currently combines a number of molecular sciences and related disciplines into seven directorates. Four directorates are focused in the core scientific areas: Chemical Structure and Dynamics, Macromolecular Structure and

Dynamics, Materials and Interfaces, and Theory, Modeling, and Simulation. Two of the directorates, Advanced Processing and Environmental Structure and Dynamics, provide a bridge between the core research areas and problem areas identified by DOE's Office of Environmental Management. Finally, one directorate, Computing and Information Sciences, provides the computing and information infrastructure for all of the EMSL.

The Office of Energy Research is currently funding a number of research activities within the interim EMSL. These efforts are supported by OHER/Health Effects and Life Sciences, OBES/Chemical Sciences, BES/Geosciences, and Mathematical, Information, and Computational Sciences/"Grand Challenge." These programs are already contributing to the development of the knowledge base needed to address DOE's environmental problems.

The EMSL will bring a significant increase in computational and modeling capabilities to PNL; these capabilities will support both ongoing and new research sponsored by OHER. The Theory, Modeling and Simulation Program and the Computer and Information Sciences Program are working with computer manufacturers to develop a high-performance computer with a design goal of approximately 1000 times the speed of a CRAY-SMP/12 for installation in the EMSL. The key role played by the EMSL staff is in the development of computational and visualization software for use on massively parallel computers, the lack of which greatly limits the usefulness of even those computers that are currently available. The Theory, Modeling, and Simulation Program is also an important new asset to the OHER programs at PNL.

**Table 5.1. Facility Construction and Modifications**

		\$M	FY
331 Complex	Install packaged boiler steam supply	0.7	1995
331 Building	Facility fire code upgrade	1.2	1995
331 Building	Convert former maintenance shop to laboratories for molecular biology research	0.4	1995
331 Building	Remove (D&D) inhalation exposure and metabolism cages	0.2	1995
331 Building	Add office wing on North side of 331	1.2	1995
331 Building	Double HEPA filter upgrade	1.5	1995
331 Building	Modification of existing laboratories to create laboratories for fundamental molecular biology research	0.7	1995
331 Building	Modification and upgrading of 1st-floor research animal facilities	2.0	1996
331 Building	Modification of 3rd-floor animal rooms to create laboratories for fundamental molecular biology research	3.0	1997
331-A Building	Remove (D&D) for upgrading 1st-floor research animal facility and Biophysics Center Construction	0.5	1996
331 Complex	Irradiation and Biophysics Center: Facility to house accelerator-based irradiation system; supporting laboratories, offices, computer shop	7.0	1995-1996
331-H	Modification to wind-tunnel building	0.6	1996
EMSL	Construction	25.2	1995
	Total	44.2	1995-1997

**Table 5.2. Examples of Major Equipment Requirements for FY 1995-1997**

Capital Equipment	Justification	\$K	FY
<b>KP-02-01</b>			
CO Analyzer	Increased sensitivity and stability for detecting manmade pollutants	25	1996
Computer workstation	Increased capability for analysis of atmospheric data	15	1996
Ozone analyzer	Faster response and sensitivity for airborne measurements on G-1	25	1996
Radiation sensors	Airborne measurements of broadband visible and infrared radiation on G-1	20	1996
Fast response humidity analyzer	Flux measurements of water vapor from surfaces	15	1997

Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
Scanning mobility particle sizer	Airborne ultrafine particle sizing and counting on G-1	38	1997
Sodar	Remote sensing of boundary layer structure	50	1997
<b>KP-02-03</b>			
Three-dimensional scanner	Dimensional analysis of physical properties of subsurface sediments	15	1995
Anaerobic glove box	Sorption/desorption experiments on ground-water chemistry	15	1995
Film recorder	Data presentation in subsurface science program	14	1995
Pulsed field electrophoresis apparatus	Restriction fragment length polymorphism studies on subsurface bacteria	20	1995
Conductivity detector	Measurements of ionized metals and organics in environmental samples	7	1995
Gel photography system	Analysis of agarose and protein gels and TLC plates	8	1995
Computer and laser printer	DNA database searches and other microbiology research applications	16	1995
Environmental chamber	Studies on chemical processes in subsurface materials	38	1995
Ultracentrifuge	Measurements of unsaturated flow properties in porous subsurface media	120	1995
<b>KP-02-04</b>			
Gas chromatograph	Detection of N <sub>2</sub> O and ethylene	30	1995
<b>KP-03-02</b>			
Fluorescence imaging system	Analysis of electrophoresis gels and blots for DNA/RNA using fluorescent labels rather than isotopes	100	1995
Applied Biosystems Stretch Upgrade for Model 373A sequencer	DNA sequencing of cloned genes	20	1995
QPCR system	Measure DNA (PCR products) in femtomole range without radiolabeling	30	1995
Applied Biosystems Model 394 DNA/RNA synthesizer	Synthesis of oligonucleotides	40	1995
Perkin Elmer thermal cycler	For PCR amplification of DNA fragments	10	1995
Zeiss Axiovert inverted microscope	For new cell culture work	20	1995
Forma Scientific Steri Culture 200 incubators (2)	For new cell culture work	12	1995

Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
IEC Centra MP4R centrifuge	Harvesting cells and nucleic acids	8	1995
Macintosh computer and accessories	DNA sequence analysis	10	1995
Beckman CE system	Separation of macromolecules	25	1995
Perkin Elmer LS-50 luminescence spectrometer	Quantification of nucleic acids	25	1995
Hewlett Packard electrospray interface for HP5989 mass spectrometer	Analysis of altered proteins and nucleic acids	100	1995
Laser densitometer	Scanning gels to quantitate amount of DNA in various bands	25	1995
Refrigerated microcentrifuge	Precipitation of DNA and RNA	19	1995
Fluorescence detector	HPLC detector to replace 15-year-old equipment	12	1995
Sun workstation	DNA sequence analysis	15	1996
Fast purification liquid chromatograph system	Rapid purification of proteins	30	1996
Perkin Elmer thermal cycler	For PCR amplification of DNA fragments	10	1996
IEC Centra MP4R centrifuge	Harvesting cells and nucleic acids	8	1996
Beckman CE system	Separation of macromolecules	25	1996
Hewlett Packard electrospray interface for HP5989 mass spectrometer	Analysis of altered proteins and nucleic acids	100	1996
Laser densitometer	Scanning gels to quantitate amount of DNA in various bands	25	1996
Fluorescence detector	HPLC detector to replace 15-year-old equipment	12	1996
Movable shelving system	Provide needed storage space for archived samples	40	1996
<b>KP-03-03</b>			
Scientific workstation	Molecular modeling	30	1995
Deflection Magnet Power Supply	Stabilization of microbeam helium ion beam	40	1996
Color printer	Representation of three-dimensional molecular structures	10	1996
<b>KP-05</b>			
140 Gbyte 8mm 10-tape stacker	Automated backup of file servers	9	1995
18 Gbyte hard disk	Additional storage for IBM workstation cluster	12	1996

Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
Two visualization workstations	Required for appropriate analysis of ocean model data	50	1996
Optical jukebox	Analysis of ocean model data	30	1996
Silicon Graphics Workstation	Support development of SGM and integrated assessment models	25	1996
Memory upgrade for workstation	Support development of SGM and integrated assessment models	8	1996
Sodar	Maintain boundary layer research capabilities	50	1997
<b>ARM Program</b>			
<b>Southern Great Plains Site</b>			
915 MHz radar wind profiler - w/RASS (3)		660	1995
AERI (2)		540	1995
Sorti		325	1995
Aerosol instruments:		42	1995
Aerosol manifold installation			
Ozone sonde		80	1995
Calibration facility		400	1995
Calibration facility instruments:			
Reference sun photometer		35	1995
Ext wavelength spectroradiometer		65	1995
Tracker		65	1995
Site data system:			
BF equipment		245	1995
Upgrade		320	1995
Racks		50	1995
Trailers for BF upgrades		40	1995
Eddy correlation system (3)		201	1995
Micro pulse lidar		100	1995
Microwave radiometer		180	1995
Whole sky imager		250	1995
Tower 25m		50	1995
EBBR		39	1996
Eddy correlation system (2)		134	1996
Microwave water vapor profiler (3)		750	1996



Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
Whole sky imager (2)		500	1996
<b>Tropical Western Pacific Site</b>			
<b>ARCS:</b>			
Control comm (AMACS)		80	1995
Generators		35	1995
Uninterrupted power supply		20	1995
<b>Instruments:</b>			
915 wind profiler		225	1995
Whole sky imaging system		250	1995
Millimeter cloud radar			
NOAA-fabrication		570	1995
Traveling wave tube (3)		225	1995
Antennas (2)		50	1995
MFRSR (7)		70	1995
Micro pulse lidar		100	1995
Microwave radiometer		120	1995
<b>SMOR</b>			
Trackers (6)		60	1995
Rad instruments (3)		36	1995
Stands/masts (2)		40	1995
<b>AERI (2)</b>		460	1995
<b>Data System:</b>			
Development sparc stations		27	1995
Network and software		45	1995
SDS hardware		225	1995
<b>ARCS:</b>			
Equipment enclosures		500	1996
Control comm (AMACS)		75	1996
Generators		35	1996
Uninterrupted power supply		40	1996
<b>Instruments:</b>			
Balloon-borne sounding system		80	1996
Whole sky imaging system		250	1996
Millimeter cloud radar			
NOAA-fabrication		570	1996
Traveling wave tube		85	1996
Antennas		25	1996
<b>MFRSR (5)</b>		50	1996
Micro pulse lidar		100	1996
Microwave radiometer		120	1996
Infrared thermometers (2)		12	1996

Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
<b>SMOR</b>			
Met instruments (2)		40	1996
Rad instruments (2)		40	1996
Stands/masts		230	1996
<b>Data System:</b>			
Network and software (2)		90	1996
SDS hardware (2)		450	1996
<b>ARCS:</b>			
Equipment enclosures (2)		1000	1997
Control comm (AMACS) (2)		150	1997
Generators (2)		70	1997
Uninterrupted power supply (3)		60	1997
<b>Instruments:</b>			
915 wind profiler (2)		450	1997
Balloon-borne sounding system		80	1997
Whole sky imaging system (2)		500	1997
Millimeter cloud radar			
NOAA-fabrication (2)		1140	1997
Travelling wave tube (2)		170	1997
Antennas (2)		50	1997
Micro pulse lidar		100	1997
Microwave radiometer		120	1997
Infrared thermometers (4)		24	1997
<b>SMOR</b>			
Trackers (3)		30	1997
Rad instruments (3)		36	1997
Stands/masts		20	1997
AERI (2)		460	1997
Microwave water vapor profiler (4)		1000	1997
<b>North Slope of Alaska Site</b>			
<b>Instruments:</b>			
Traveling wave tube		85	1995
Micro pulse lidar		100	1995
AERI		325	1995
<b>Experiment center equipment:</b>			
Completion of upgrade		150	1995
<b>Archive</b>		1100	1995
<b>ARCS:</b>			
Equipment enclosures (2)		700	1996
Control comm (AMACS) (2)		125	1996
Generators		35	1996
Uninterrupted power supply (2)		40	1996

Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
<b>Instruments:</b>			
449 wind profiler		500	1996
Balloon-borne sounding system		80	1996
Whole sky imaging system (2)		500	1996
Millimeter cloud radar			
NOAA - fabrication		570	1996
Traveling wave tube		85	1996
Antennas (2)		50	1996
MFRSR (4)		40	1996
Micro pulse lidar		100	1996
Microwave radiometer (2)		240	1996
Infrared thermometer (4)		24	1996
<b>SMOR:</b>		20	1996
Trackers/stands/masts (2)		40	1996
Met instruments (2)		48	1996
Rad instruments (2)		325	1996
<b>AERI</b>			
<b>Data system:</b>			
Development sparc stations		27	1996
Network and software (2)		90	1996
SDS hardware (2)		450	1996
<b>Experiment center equipment:</b>			
Completion of upgrade		150	1996
<b>Archive</b>		100	1996
<b>ARCS:</b>			
Generators		70	1997
<b>Instruments:</b>			
449 wind profiler		500	1997
Balloon-borne sounding system		80	1997
Whole sky imaging system (2)		500	1997
Millimeter cloud radar			
NOAA - fabrication		570	1997
Traveling wave tube		85	1997
Antennas		25	1997
MFRSR (2)		20	1997
Micro pulse lidar		100	1997
Microwave radiometer		120	1997
Infrared thermometer (4)		24	1997

Table 5.2. (contd)

Capital Equipment	Justification	\$K	FY
SMOR:			
Trackers/stands/masts		10	1997
Met instruments		20	1997
Rad instruments (2)		24	1997
AERI		300	1997
SORTI		375	1997
Microwave water vapor profiler		250	1997
Raman-lidar		700	1997
Data system			
Network and software		45	1997
SDS hardware		225	1997
Experiment center equipment			
Completion of upgrade		300	1997
Archive		200	1997
Instrumentation for Clusters and Surfaces		1,630	1995
Electronic Structure Spectroscopic Laser System		110	1995
Auger Electron Spectrometer/Scanning Auger Microscope		1,063	1995
Secondary Ion Mass Spectrometer		1,014	1995
Fourier Transform Electron Paramagnetic Resonance Spectrometer		750	1994
Ultrahigh Resolution Scanning Electron Microscope		666	1995
Chemical Vapor Deposition System		578	1995
Molecular Beam Epitaxy System		465	1995
Research Epitaxy System		1,565	1995
23-Tesla Magnet		7,992	1994
RF System and Console		713	1994
Superconducting Magnet		2,242	1994
High Performance Computer System		1,842	1994
Graphics and Visualization Laboratory		164	1995
Code Development Workstations		300	1994
Code Development Workstations		130	1995
Network Infrastructure		145	1994
Network Infrastructure		348	1995
Distributed Computing Systems		133	1995
Distributed computing Systems			

**Table 5.2. (contd)**

<b>Capital Equipment</b>	<b>Justification</b>	<b>\$K</b>	<b>FY</b>
IDL-Design and Development Support		200	1995
IDO-Design and Development Support			
Database Computer System		705	1994

## **6.0 Contemporary Issues**

### **6.1 Capital Equipment Funds**

The capital equipment fund allocation for all non-ARM projects has been \$200K for each of the past two years. This amount of capital dollars for a programmatic funding base of over \$20M is inadequate to support modern environmental and health-related research. The \$200K does not allow modernization of existing equipment, much less provide for new equipment to conduct research which is becoming more capital intensive. A capital allocation in the range of 10% of the programmatic base is more in line with what is needed to sustain modern research where we are studying more complex, real-world systems. If the pool of funds available for capital purchases cannot be increased, it would be helpful for DOE to raise the ceiling on capital purchases from the current level of \$5000. In this manner, a scientist could have the freedom to purchase a major piece of equipment as opposed to funding a postdoctoral associate. There are times when some capital equipment would make the research more productive than another pair of hands.

### **6.2 Environmental Molecular Sciences Laboratory**

The completion of the EMSL project and the development of new research programs to take advantage of the new capabilities offered by the EMSL is a major issue for PNL. In developing the research programs for the EMSL it is important that we maintain our current strong OHER-sponsored research at PNL. Our ongoing research in health effects, subsurface science, global change, and biotechnology is necessary to provide the problem sets, identify the key scientific issues that molecular science can solve, and supply the physiochemical and biological systems that we will study in the EMSL. Our aim is to infuse the new EMSL capital investments into all our OHER research programs, thereby helping to relieve some of the need for major capital funds described above.

### **6.3 Program Integration**

At PNL we are pursuing more integration and synergy within all programs sponsored by OER (OHER, BES, and MICS) with the goal of coupling the knowledge output for our programs with the needs of DOE's environmental programs. This program integration and focusing of research to attack select problem sets requires some degree of flexibility from both our scientists and the program managers. In particular, the knowledge base and time frame for solutions from the EM perspective is often much different from that of OHER. Frequent communication between PNL, DOE-RL, and DOE-HQ is required if all parties are to develop and sustain a relationship where the research sponsored by OHER is recognized by EM as providing solutions to their environmental restoration and waste management problems.

## 7.0 Appendices

### 7.1 Staffing by Program Area

This year's Director's Overview presents the staffing information by budget category rather than department, which differs from the format used in previous years. These numbers more accurately reflect the Program.

#### KP-01: OHER Personnel

	Full-Time Equivalents <sup>(a)</sup>		
	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
Professional (Scientific)	2	2	2
Postdoctorates	4	4	4
Technicians	0	0	0
Animal Care	0	0	0
<b>Total Direct Personnel</b>	<b>6</b>	<b>6</b>	<b>6</b>
Professional (Adm.)	0	0	0
Clerical, Adm. Support	1	1	1
Maintenance	0	0	0
<b>Total Indirect Personnel</b>	<b>1</b>	<b>1</b>	<b>1</b>
Visiting Scientists	0	0	0
Graduate Students	0	0	0
Undergraduates	0	0	0
High School Students	0	0	0

#### KP-01: OHER Staff by Degrees<sup>(c)</sup>

Degree	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
BS/BA	0	0	0
MS	1	1	1
PhD	5	5	5
DVM	0	0	0
ND	1	1	1

**KP-02: OHER Personnel**

	Full-Time Equivalents <sup>(a)</sup>		
	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
Professional (Scientific)	45	46	46
Postdoctorates	0	0	0
Technicians	6	6	6
Animal Care	0	0	0
<b>Total Direct Personnel</b>	<b>51</b>	<b>52</b>	<b>52</b>
Professional (Adm.)	15	15	15
Clerical, Adm. Support	5	5	5
Maintenance	0	0	0
<b>Total Indirect Personnel</b>	<b>20</b>	<b>20</b>	<b>20</b>
Visiting Scientists	0	0	0
Graduate Students	0	0	0
Undergraduates	0	0	0
High School Students	0	0	0

**KP-02: OHER Staff by Degrees<sup>(c)</sup>**

Degree	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
BS/BA	10	10	10
MS	14	14	14
PhD	35	36	36
DVM	0	0	0
ND	12	12	12



**KP-03: OHER Personnel**

	Full-Time Equivalents <sup>(a)</sup>		
	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
Professional (Scientific)	16	10	12
Postdoctorates	2	0	0
Technicians	1	2	3
Animal Care	<u>3</u>	<u>1</u>	<u>0</u>
<b>Total Direct Personnel</b>	<b>22</b>	<b>13</b>	<b>15</b>
Professional (Adm.)	4	1	1
Clerical, Adm. Support	1	1	1
Maintenance	<u>2</u>	<u>0</u>	<u>0</u>
<b>Total Indirect Personnel</b>	<b>7</b>	<b>2</b>	<b>2</b>
Visiting Scientists	2	0	0
Graduate Students	2	0	0
Undergraduates	1	1	1
High School Students	0	0	0

**KP-03: OHER Staff by Degrees<sup>(c)</sup>**

Degree	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
BS/BA	4	4	4
MS	5	1	1
PhD	17	10	12
DVM	1	0	0
ND	2	1	1

**KP-04: OHER Personnel**

	Full-Time Equivalents <sup>(a)</sup>		
	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
Professional (Scientific)	2	2	2
Postdoctorates	2	5	6
Technicians	0	0	0
Animal Care	0	0	0
<b>Total Direct Personnel</b>	<b>4</b>	<b>7</b>	<b>8</b>
Professional (Adm.)	0	0	0
Clerical, Adm. Support	1	1	0
Maintenance	0	0	0
<b>Total Indirect Personnel</b>	<b>1</b>	<b>1</b>	<b>0</b>
Visiting Scientists	1	1	2
Graduate Students	2	2	3
Undergraduates	0	1	0
High School Students	0	0	0

**KP-04: OHER Staff by Degrees<sup>(c)</sup>**

Degree	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
BS/BA	0	1	1
MS	2	2	2
PhD	2	2	2
DVM	0	0	0
ND	1	1	1

**KP-05: OHER Personnel**

	Full-Time Equivalents <sup>(a)</sup>		
	FY 1993	FY 1994	FY 1995 <sup>b</sup>
<b>Non-ARM</b>			
Professional (Scientific)	22	25	25
Postdoctorates	4	4	4
Technicians	3	3	3
Animal Care	0	0	0
<b>Total Direct Personnel</b>	<b>29</b>	<b>32</b>	<b>32</b>
Professional (Adm.)	3	4	4
Clerical, Adm. Support	2	2	2
Maintenance	0	0	0
<b>Total Indirect Personnel</b>	<b>5</b>	<b>6</b>	<b>6</b>
Visiting Scientists	5	5	5
Graduate Students	9	10	10
Undergraduates	1	1	1
High School Students	2	2	2
<b>ARM Program</b>			
<b>Atmospheric Radiation Measurement (ARM Program)</b>			
Professional (Scientific)	24	28	28
Technicians	0	0	0
<b>Total Direct Personnel</b>	<b>24</b>	<b>28</b>	<b>28</b>
Professional (Adm.)	7	8	8
Clerical, Adm. Support	4	4	4
Maintenance	0	0	0
<b>Total Indirect Personnel</b>	<b>11</b>	<b>12</b>	<b>12</b>

**KP-05: OHER Staff by Degrees<sup>(c)</sup>**

	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
BS/BA	33	40	40
MS	6	6	6
PhD	20	22	22
DVM	0	0	0
ND	10	10	10

**Summary Table for All OHER Personnel (includes OHER Management Personnel)**

	Full-Time Equivalents <sup>(a)</sup>		
	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
Professional (Scientific)	112	120	120
Postdoctorates	12	12	13
Technicians	10	10	10
Animal Care	3	2	2
<b>Total Direct Personnel</b>	<b>137</b>	<b>144</b>	<b>145</b>
Professional (Adm.)	30	32	32
Clerical, Adm. Support	14	14	14
Maintenance	2	2	2
<b>Total Indirect Personnel</b>	<b>46</b>	<b>48</b>	<b>48</b>
Visiting Scientists	8	8	9
Graduate Students	13	13	14
Undergraduates	2	1	1
High School Students	2	2	2

**OHER Staff by Degrees<sup>(c)</sup>**

Degree	FY 1993	FY 1994	FY 1995 <sup>(b)</sup>
BS/BA	49	57	57
MS	29	26	26
PhD	81	84	84
DVM	1	1	1
ND	26	26	26

(a) In FY 1993, \$9.7M (~30%) and in FY 1994 and FY 1995, \$10M (~35%) of PNL's OHER budget, primarily in the ARM Program, is for subcontracts with other organizations. The numbers in this table do not include staff working on those subcontracts.

(b) FY 1995 is estimated.

(c) OHER-sponsored scientific professionals by highest degree attained. Discrepancies between totals may result from the differences between FTEs and actual assigned personnel. These data do not reflect many degreed scientists from throughout PNL who work part-time on OHER programs.

Key: BA = Bachelor of Arts; BS = Bachelor of Science; MS = Master of Science; PhD = Doctor of Philosophy; DVM = Doctor of Veterinary Medicine; ND = No degree.

## 7.2 Information Transfer

	OHER-Sponsored Research	
	FY 1993	FY 1994
Journal Articles (peer-reviewed)	67	109
Chapters, Reviews	0	0
Books/Proceedings	47	25
Reports/Documents	10	8
Presentations at Technical Meetings	241	225
Meetings Organized <sup>(a)</sup>	16	5
Nonlaboratory Users/Number of Days Used OHER Facilities <sup>(b)</sup>	-	-
Thesis	1	0

(a) See Section 7.3 for detail.

(b) Totals for participants in user facilities are not available. A brief description of the total facilities used for OHER research is given in Table 2.3. Most of these facilities are available for use by nonstaff researchers who qualify for access to the Hanford Site.

## 7.3 Conferences, Workshops, and Training Programs

Title	Date	PNL Organizer/ Participant
Local Organizer/Participant, ICRP Task Group on Internal Dosimetry (INDOS), Richland, Washington	November 1993	FT Cross
Co-Chairman, Symposium on Radon at the 24th Annual Meeting of the European Society for Radiation Biology, Erfurt, Germany	October 1992	GE Dagle
Chairman, ASCOT Science Meeting, Salt Lake City, Utah	February 1993	JC Doran
Co-chair of XIV International Seminar on Ion Atom Collisions		RD DuBois
Future Prospects for Medical Isotopes at Hanford and the Tri-Cities	March 17, 1995	TS Tenforde
Hanford's Medical Isotopes Program	April 21, 1995	TS Tenforde
Co-Chairman, Workshop Radiation Damage in DNA: Structure/Function Relationship at Early Times	October 1994	AF Fuciarelli
Co-Chairmen, Hydrology Days Special - Flow in Heterogeneous Porous Media, American Geophysical Union	March 1993	GW Gee
Session Chairman, 32nd Hanford Symposium on Health and the Environment	November 1993	SJ Ghan
Chairperson, Workshop on Background Aerosols and Visibility	June 1993	NL Laulainen
Chairman, 31st Hanford Symposium on Health and Environment	October 1992	LE Sever

## 7.4 Extramural Activities

Who	What
<b>Awards and Honors</b>	
DR Fisher	AWU/DOE Laboratory Distinguished Lecturer
AF Fuciarelli	Young Investigator Award to attend the 18th L. H. Gray Conference on Radiation Damage in DNA Physics, Chemistry and Molecular Biology, University of Bath, United Kingdom, April 1994
<b>Committees</b>	
LE Anderson	Member, US/USSR Cooperative Scientific Committee on Biological Effects of Physical Factors in the Environment  Member, U.S. delegation, Commission K, Union of Radio Science Internationale (URSI)  Member, National Council on Radiation Protection (NCRP) Scientific Committee SC-89-3, Extremely Low Frequency Electric and Magnetic Fields  Member, National Academy of Sciences (NAS)/National Research Council Committee on Biological Effects of Electromagnetic Fields
WE Asher	Member, Organizing Committee for the Third International Symposium on Air/Water/Gas Transfer
WR Barchet	US-Canadian Model Evaluation Team
LA Braby	Member, Science and Technology Consultant Pool of Committee on Interagency Radiation Research and Policy Coordination (CIRRPC), Committee on High-LET Radiobiology  Committee, 1994 Workshop on Microdosimetry  Member, NCRP Committee 88 on fluence as a basis of a system of radiation protection for astronauts  Member, European Radiation Dosimetry Group (EURADOS) Working Group 10, "Basic Physical Data and Characteristics of Gas Ionization Devices"  Member, NCRP
F Brockman	Member, Organizing Committee, 33rd Hanford Symposium on Health and the Environment, <i>In Situ Remediation: Scientific Basis for Current and Future Technologies</i>
AL Brooks	Chairman, NCRP Committee 57-Subcommittee II, "Liver Cancer Risk"  Member, NCRP; Member, NCRP Scientific Committee 83, Research Needs for Setting Radiation Standards  Member, NIH/NCI Council, Biology, Immunology Contract Review Committee
FT Cross	Member, NCRP  Member, NCRP Scientific Committee 85 on Radon Risk  Member, ICRP Committee 2 on Derived Limits

Who	What
<b>Committees (contd)</b>	
FT Cross (contd)	<p>Member, Technical Review Panel, Atomic Energy Control Board of Canada</p> <p>Chairman, Health Effects Committee of DOE/Commission of the European Communities (CEC) Radon Risk Report</p> <p>Member, Washington State Radon Health Effects Committee</p> <p>Member, Science &amp; Technology Consultant Pool of CIRRPC</p> <p>Member, Graduate Research Committee, Washington State University</p>
JC Doran	<p>Member, ARM Science Team Executive Committee</p> <p>Member, Mountain Meteorology Committee, American Meteorological Society</p>
RJ Douthart	<p>Member, Advisory Board on Visualization and Design in Molecular Sciences (VADMS), Washington State University</p> <p>Member, Biotechnology Advisory Committee, Rensselaer Polytech Institute</p>
JP Downing	<p>Working Group Leader: Land and Water Interfaces International Workshop on Terrestrial Biospheric Carbon Fluxes: Quantification of Sinks and Sources of CO<sub>2</sub></p> <p>Technical Director, DOE CO<sub>2</sub> Survey Science Team</p> <p>Chairman, Ocean Measurements Working Group, ARM Program</p>
RD DuBois	<p>Consultant, International Commission on Radiological Units (ICRU) Report Committee on Ion-Induced Electron Spectra</p>
JA Edmonds	<p>Lead Author, Intergovernmental Panel on Climate Change (IPCC) Working Group II: Energy Supply Mitigation Strategies writing team</p> <p>Lead Author, IPCC Working Group III: Emissions Scenarios writing team</p> <p>Testimony before House Committee on Energy and Commerce: Edmonds, J., "Greenhouse Gases and Human Activities," Statement before the Subcommittee on Energy and Power, United States House of Representatives, March 10, 1993, Washington, DC</p> <p>Testimony before Senate Committee on Energy and Natural Resources: Edmonds, J., "Greenhouse Gases and Human Activities," Statement before the Committee on Energy and Natural Resources, United States Senate, March 30, 1993, Washington, DC</p> <p>Member, Electric Power Research Institute (EPRI) Global Climate Advisory Board</p>
RA Elston	<p>Chairman, Committee on Shellfish Diseases, Washington State Department of Fisheries</p> <p>Member, Department of Commerce "Ninth Working Group on U.S.-Canada Trade and Tariff Negotiations on Fishery Products"</p> <p>Washington Aquaculture Advisory Council</p> <p>Member, Pacific Northwest Fish Health Protection Committee</p> <p>Member, three graduate research committees, University of Washington</p>

Who	What
<b>Committees (contd)</b>	
DR Fisher	Chairman, NCRP Scientific Committee 46-10 on Assessment of Occupational Dose from Internal Emitters  Member, Medical Internal Radiation Dose Committee of the Society of Nuclear Medicine  Member, American National Standards Institute/Health Physics Society Working Group N13.39 on Internal Dosimetry
JK Fredrickson	Member, Organizing Committee, Second International Symposium on Subsurface Microbiology  Chair-elect, Division N - Microbial Ecology for American Society of Microbiology, 1996 Annual Meeting
AF Fuciarelli	Chairman, Radiation Research Society Education and Training Committee
GW Gee	Past Chairman, Division S1 (Soil Physics), Soil Science Society of America  Member, D-18 (Soil and Rock), American Society for Testing and Materials  Member, W155, Western Regional Research Committee on Flow/Transport in Soils at the Field Scale  Member, Hanford Science Symposium Planning Committee
ES Gilbert	Member, NAS Advisory Committee for Epidemiological Study of Crossroads Participants  Member, NCRP  Member, Committee on Health Risk of Exposure to Radon (BEIR VI)
TR Ginn	Member, ASCE Task Committee to Review Probabilistic Methods of Subsurface Transport
BJ Greenspan	Secretary, ANSI 288.12 Committee on Respiratory Protection for Infectious Aerosols
AC James	Member, Project Review Committee, American Water Works Association  Member, Technical Review Panel, Atomic Energy Control Board of Canada
NS Laulainen	US-Canadian Diagnostic Measurement Team for Regional Model Evaluation
RJ Lenhard	Chairman, Unsaturated Zone Committee of the American Geophysical Union
SO Link	Member, Benton County Noxious Weed Control Board  Member, National Steering Panel for Protective Barrier Studies  Member, Pacific Northwest Exotic Pest Plant Council  Member, Western Weed Coordinating Committee  Member, Shrub Research Consortium Governing Board  Member, International Advisory Board of the Japanese Association for Arid Land Studies  Adjunct Faculty Member, Washington State University
RH Lovely	Member, NCRP Scientific Committee 89-3 on ELF Electric and Magnetic Fields



Who	What
<b>Committees (contd)</b>	
DD Mahlum	Chairman, NCRP Scientific Committee 89-1 on Biological Effects of Magnetic Fields Member, Advisory Committee on Environmental Toxicology, Florida A&M University Member, Minority Institutions Advisory Committee, Florida A&M University
PW Mellick	Member, Respiratory Tract Panel, Armed Forces Institute of Pathology Registry of Toxicologic Pathology
DL Miller	Member, NCRP Committee 66 on Biological Effects of Ultrasound Member, Acoustical Society of America Standards Committee Working Group 22
RL Ornstein	Member, NIH Special Study Section in Physical Biochemistry
JF Park	Member, Interagency Nuclear Safety Review Panel for NASA Cassini Mission Member, BEES Subpanel, Interagency Nuclear Safety Review Panel
WT Pennell	Member, Committee on the Meteorological Aspects of Air Pollution, American Meteorologic Society
LE Rogers	Member, Association Ecological Research Center Advisory Panel
JD Shaffer	Radiation Study Section, NIH
RJ Serne	Member, International Atomic Energy Agency (IAEA) Committee on Nuclear Technologies Studying Pollutant Transport in the Environment Member, ICRP Task Group on Age-Dependent Dosimetry and Dose per Unit Intake for Members of the Public
LE Sever	Member, Advisory Committee, National Institute on Drug Abuse, The National Pregnancy and Health Study Member, Professional Advisory Council, Spina Bifida Association of America President ProTem, Washington State Genetic Advisory Committee Chairman, Health Professional Advisory Committee, Western Washington Chapter, March of Dimes Birth Defects Foundation Member, Executive Committee, Western Washington Chapter, March of Dimes Birth Defects Foundation Member, Data Committee, Pacific Northwest Regional Genetics Group Member, Educational Committee, Pacific Northwest Regional Genetics Group
WJ Shaw	Member, AMS Committee on Meteorology and Oceanography of the Coastal Zone
CR Sherwood	Rapporteur of Coastal Oceanography Program (COOP) Working Group in Portland

Who	What
<b>Committees (contd)</b>	
MR Sikov	<p>Member, Advisory Board of Outlook; Program for the Introduction and Adaptation of Contraceptive Technology (PIACT)</p> <p>Chairman, NCRP Scientific Committee 57-14 on Placental Transfer of Radionuclides</p> <p>Corresponding member, ICRP Task Group on Age-Dependent Dosimetry of Radionuclides</p>
DL Springer	Member, American Water Works Association Research Division Committee on Health Effects
RG Stevens	Member, NCRP Committee 89-3 on ELF Electric and Magnetic Fields
TS Tenforde	<p>Member, Institute of Electrical and Electronics Engineers Standards Coordinating Committee 28 on Nonionizing Radiation</p> <p>Member, NCRP; Member, NCRP Scientific Committee 89-1 on Biological Effects of Magnetic Fields; Member, NCRP Nominating Committee; Member, NCRP Board of Directors; Chairman, NCRP Committee 89 on Nonionizing Electromagnetic Fields; Member, NCRP Committee 1 on Radiobiology, Risk and Basic Radiation Protection</p> <p>Member, American Conference of Governmental Industrial Hygienists, Physical Agents TLV Committee</p> <p>Member, National Research Council Board on Radiation Effects Research</p> <p>Member, International Commission on Nonionizing Radiation Protection of the International Radiation Protection Association</p> <p>Member, Harvard Center for Risk Analysis Advisory Committee on Electromagnetic Fields and Human Health</p>
JM Thomas	Member, Review Panel for EPA's Landscape Ecology Research Program
CR Watson	Member, Committee on Automated Record Technology, Society of American Archivists
RE Weller	Member, two graduate research committees, Washington State University
CD Whiteman	<p>Member, Committee on Mountain Meteorology, AMS</p> <p>Member, U.S. Forest Service (USFS) National Spray Advisory Committee</p> <p>Member, Technical Review Committee, Brown Cloud II Project</p> <p>Member, National Spray Model and Application Technology Committee</p> <p>Member, Tethered Balloon Technology Development Consortium</p> <p>Member, International Committee to Plan Research for the Mesoscale Alpine Programme (MAP). Leader of the Working Group on Boundary Layer Processes, Thermally Driven Circulations and Atmospheric Tracers, MAP Planning Meeting, Zurich, Switzerland, September 12-16, 1994</p>

Who	What
<b>Committees (contd)</b>	
RE Wildung	<p>Member, Scientific Advisory Council, Glenn T. Seaborg Institute for Transactinium Science</p> <p>Member, Clemson University Advisory Committee for College of Agriculture</p> <p>Member, Advisory Committee for College of Agriculture</p> <p>Chairman, Soil Contamination Task Group, NCRP Scientific Committee 64</p> <p>Member, DOE/OHER Directors Council, Environmental Research Park Program</p> <p>Member, Awards Committee, American Society of Agronomy/Soil/Science Society of America</p> <p>Member, Board of Visitors, College of Sciences, Washington State University</p>
JM Zachara	<p>Member, American Geophysical Union, Groundwater Hydrology Advisory Panel</p> <p>Member, Organizing Committee, Second International Symposium on Subsurface Microbiology</p> <p>Member, Clay Minerals Society</p> <p>Member, American Chemical Society</p> <p>Member, Geochemical Society</p> <p>Member, Stanford Synchrotron Radiation Laboratory Peer Review Panel</p> <p>Principal Scientist and Coordinator, DOE/OHER Subsurface Science Program Research in Co-Contaminant Chemistry</p> <p>Associate Editor, Journal of Contaminant Hydrology</p>
<b>Consultant Work and University Appointments</b>	
LE Anderson	<p>Adjunct Faculty Appointment, Washington State University-Tri-Cities</p> <p>Reviewer, EPRI scientific review teams</p>
DK Blough	<p>Adjunct Faculty, Washington State University</p> <p>Program Coordinator, Mathematics and Statistics, Washington State University</p>
H Bolton	Adjunct Professor, Washington State University
LA Braby	Program Review committee member for DOE/OHER and NIH
FJ Brockman	<p>Adjunct Faculty Appointment, Washington State University</p> <p>Associate Faculty Member, Department of Environmental and Civil Engineering, Washington State University</p>
AL Brooks	Adjunct Faculty Appointment, Washington State University
FT Cross	Consultant to Atomic Energy Control Board of Canada on health effects in uranium miners from high-grade uranium ore

Who	What
<b>Consultant Work and University Appointments (contd)</b>	
	Consultant to DOE, CEC, EPA, BPA, NCRP, NAS, state agencies, and private industry on health effects of radon
	Adjunct Lecturer, Washington State University
GE Dagle	Lecturer, Program in Biology, Washington State University-Tri-Cities
RJ Douthart	Adjunct Professor, Washington State University
RA Elston	Adjunct Professor, University of Washington
	Adjunct Professor, Washington State University
	Shellfish Resource Management Advisor to Washington State Department of Fisheries
DR Fisher	Affiliate Assistant Professor of Radiology, University of Washington School of Medicine
	Affiliate Assistant Professor, Environmental Health, University of Washington School of Public Health
	Adjunct Assistant Professor, Nuclear Engineering, Texas A&M University
	Adjunct Lecturer, Environmental Sciences and Regional Planning, Washington State University-Tri-Cities
	Affiliate Investigator, Division of Clinical Research, Fred Hutchinson Cancer Research Center
JK Fredrickson	Adjunct Professor, University of Idaho
	Adjunct Professor, Washington State University
AF Fuciarelli	Lecturer, Washington State University
	Member of NIH Special Review Committee (ad hoc): "The Regulation, Function and Specificity of Proteins Induced in Mammalian Cells Exposed to Ionizing Radiation"
GW Gee	Special American Business Internship Training (SABIT) Collaborator, U.S. Department of Commerce, Former Soviet Scientist Exchange
	IAEA Collaborator, IAEA Fellowship Program, Vienna, Austria
	Graduate Advisor/Adjunct Professor, Washington State University and University of Idaho
	Graduate Advisor, University of Washington
	Collaborator, Desert Research Institute, Reno, Nevada
	Collaborator, U.S. Geological Survey, Tacoma, Washington; Carson City, Nevada
SJ Ghan	Adjunct Associate Professor, University of Washington
TE Hui	Consultant, Fred Hutchinson Cancer Research Center
	Consultant, City of Hope National Medical Center
AC James	Consultant to Atomic Energy Control Board of Canada on health effects of high-grade uranium ore

Who	What
<b>Consultant Work and University Appointments (contd)</b>	
AC James (contd)	<p>Consultant and Expert Witness for British Nuclear Fuels PLC, England, on dose to the testes of Ontario uranium miners from exposure to radon and uranium ore</p> <p>Consultant, Department of Minerals and Energy, W. Australia, on implications of new ICRP lung model for mineral sands industry</p> <p>Consultant, South African Association of Physicists in Medicine and Biology and Presenter of Summer School in Radiation Protection, Allemanskraal Dam</p>
FC Leung	Adjunct Professor at Washington State University, University of Washington, Eastern Washington State University, and University of Idaho
SO Link	Adjunct Faculty Member, Washington State University
TJ Mast	<p>Member, Graduate Faculty, Toxicology Program, Oregon State University</p> <p>Adjunct Associate Professor of Pharmacology, Toxicology Department, Washington State University</p>
JP McKinley	Adjunct Lecturer, Washington State University
RJ Miller	Adjunct Professor and Visiting Lecturer, Whitman College, Walla Walla, Washington
PE Long	Member, Richland School District Science Committee
RL Ornstein	<p>Adjunct Professor, Chemistry Department, Washington State University</p> <p>Visiting Research Professor, Department of Biophysics, Roswell Park Cancer Institute</p> <p>Consultant, Darwin Molecular</p> <p>Consultant, Environmental Health Science Center, University of Arizona-Tucson</p>
HA Ragan	Member, Graduate Faculty, Biology Department, Washington State University
RA Renne	Guest Lecturer, Washington State University-Tri-Cities
WH Rickard	Adjunct Professor, Washington State University
LE Rogers	Adjunct Professor, Washington State University
LB Sasser	<p>Adjunct Faculty Member, Washington State University</p> <p>Consultant, Fred Hutchinson Cancer Research Center</p>
LE Sever	<p>Member, Graduate Faculty, University of Washington</p> <p>Affiliate Professor, Department of Epidemiology, University of Washington School of Public Health and Community Medicine</p> <p>Affiliate Professor, Department of Environmental Health, University of Washington School of Public Health and Community Medicine</p> <p>Faculty, New England Epidemiology Summer Program, New England Epidemiology Institute/Tufts University</p> <p>Center Affiliate, Center for Women's Health Research, University of Washington School of Nursing</p>

Who	What
<b>Consultant Work and University Appointments (contd)</b>	
W Shaw	Adjunct Associate Professor of Environmental Sciences at Washington State University, Tri-Cities
MR Sikov	Program Consultant, Atomic Energy Control Board of Canada, Transport of Compounds from Mother to Foetus
RD Smith	Distinguished Lectureship, AWU/DOE Affiliate Faculty Member, University of Idaho Adjunct Professor, Washington State University
DL Springer	Adjunct Associate Professor of Toxicology, College of Pharmacy, Washington State University Graduate Faculty Member, Toxicology Program, Oregon State University
RG Stevens	Clinical Associate Professor, Department of Epidemiology, University of Washington
TS Tenforde	Board of Directors, Lanzl Institute of Medical Dosimetry, Seattle, Washington
JM Thomas	Adjunct Professor, Washington State University Member, Ecological Advisory Subcommittee of the Science Advisory Board, Washington State Department of Ecology
RE Weller	Adjunct Professor, Tuskegee University Consultant, Pan American Health Organization Coordinator, World Health Organization Collaborative Center for Training and Reference in Clinical Pathology of Neotropical Primates Adjunct Lecturer, Program in Biology, Washington State University Coordinator, Biology Program, Washington State University Tri-Cities Campus
CD Whiteman	Adjunct Associate Professor, Washington State University Member, Graduate Faculty, Washington State University Visiting Scientist, Paul Scherrer Institut, Villigen, Switzerland, August 1-October 31, 1994 Visiting Dozent Professor, Geographical Institute, University of Bern, Switzerland, November 7, 1994-February 7, 1995 Adjunct Associate Professor of Environmental Science, Washington State University, Pullman, Washington, FY 1994 to present Visiting Professor of Geography, University of Berne, Switzerland, November 1994 through June 1995
RE Wildung	Adjunct Professor, Washington State University Board of Visitors, Washington State University, Pullman, Washington

Who	What
<b>Consultant Work and University Appointments (contd)</b>	
BW Wilson	Consultant, U.S. Coast Guard Civil Engineering Unit Consultant, Puget Sound Power and Light Company Consultant, Seattle City Light Company
WE Wilson	Affiliate Associate Professor, University of Washington Adjunct Lecturer, Washington State University
JM Zachara	Graduate Advisor, University of Florida
<b>Editorial Board Memberships</b>	
LE Anderson	Associate Editor, <i>Bioelectromagnetics</i>
CE Cushing	Member, Editorial Board, North American Benthological Society (national) Book Review Editor, North American Benthological Society
RA Elston	Associate Editor, <i>Journal of World Aquaculture Society</i> Member, Editorial Board of the following journals: <i>Diseases of Aquatic Organisms</i> , <i>Journal of Invertebrate Pathology</i> , <i>Journal of Shellfish Research</i> , <i>Journal of Fish Diseases</i> , and <i>Fish and Shellfish Immunology</i>
DR Fisher	Associate Editor, <i>Antibody Immunoconjugates and Radiopharmaceuticals</i>
JK Fredrickson	Member, Editorial Board of the following journals: <i>Microbial Ecology and Applied and Environmental Microbiology</i> Editor-in-Chief, <i>Microbial Ecology</i>
SJ Ghan	Member, Editorial Board of the following journals: <i>Climatic Change and Encyclopedia of Weather and Climate</i>
TR Ginn	Associate Editor, <i>Stochastic Hydrology and Hydraulics</i> Associate Editor, <i>Water Resources Research</i>
EA Jenne	Member, Editorial Board, <i>Chemical Speciation and Bioavailability</i>
DD Mahlum	Member, Editorial Board, <i>Toxicology</i>
DL Miller	Member, Editorial Board, <i>Ultrasound in Medicine and Biology</i>
RL Ornstein	Associate Editor, <i>Journal of Biomacromolecular Structure &amp; Dynamics</i>
SA Rawson	Member, Editorial Board, <i>Geology</i>
WGN Slinn	Board of Editors, <i>Tellus Series B Chemical and Physical Meteorology</i> , Swedish Geophysical Society Associate Editor, <i>Atmospheric Environment</i>
RD Smith	Member, Editorial Board of the following journals: <i>Journal of Supercritical Fluids</i> , <i>Journal of Microcolumn Separations</i> , <i>Journal of Capillary Electrophoresis</i> , and <i>Biological Mass Spectrometry</i>

Who	What
<b>Editorial Board Memberships (contd)</b>	
TS Tenforde	Member, Editorial Board, <i>Bioelectromagnetics</i>
RE Weller	Member, Editorial Board of the following journals: <i>Journal of Medical Primatology</i> , <i>Journal of Veterinary Internal Medicine</i> , and <i>Journal of the American Veterinary Medical Association</i>
BW Wright	Member, Editorial Board, <i>Journal of Microcolumn Separations</i>
JM Zachara	Member, Editorial Board, <i>Journal of Contaminant Hydrology</i>
<b>Societies-Committee Service</b>	
LE Anderson	Chairman, Strategic Planning Committee, Bioelectromagnetics Society Chairman, Bioelectromagnetics Society Awards Committee Member, Bioelectromagnetics Society, Public Policy and Advocacy Committee
RA Elston	Member, Executive Committee, National Shellfisheries Association Member, Site Selection Committee, National Shellfisheries Association Member, Elections Committee, National Shellfisheries Association Member, Membership Committee, Society for Invertebrate Pathology
AF Fuciarelli	Chair-Education and Training Committee-Radiation Research Society
GW Gee	Newsletter Editor, Division S1, Soil Science Society of America
RF Jostes	Member, Membership Committee, Radiation Research Society
SV Mattigod	Chairman, Necrology Committee, American Society of Agronomy and Soil Science Society of America
JD Saffer	Education and Outreach Committee, Bioelectromagnetics Society Annual Meeting Committee, Bioelectromagnetics Society
LE Sever	Program Committee, Society for Pediatric Epidemiologic Research
TS Tenforde	Chairman, Technical Program Committee for 1994 NCRP Annual Meeting
CD Whiteman	Chairman, National Spray Model Advisory Committee Member, Mountain Meteorology Committee, AMS
<b>Societies-Offices Held</b>	
BJ Chou	Secretary, Chinese-American Toxicology Society
RA Elston	President, National Shellfisheries Association
AF Fuciarelli	Chairman, Radiation Research Society Education and Training Committee
JM Nelson	President, Local Chapter Sigma Xi President, Cell Kinetics Society



Who	What
<b>Societies-Offices Held (contd)</b>	
WH Rickard	Governing Board, Northwest Scientific Association
JD Saffer	Member, Board of Directors, Bioelectromagnetics Society
DL Springer	President, Pacific Northwest Association of Toxicologists, a chapter of the Society of Toxicology
RE Weller	Treasurer, Veterinary Cancer Society
	Member, Executive Committee, Veterinary Cancer Society
	Member, Board of Reviewers, American Veterinary Medical Association
	Chairman, Examination Committee, Specialty of Veterinary Medical Oncology, American College of Veterinary Internal Medicine
BW Wilson	Chairman, Development Committee, Bioelectromagnetics Society
	Member, Board of Directors, Bioelectromagnetics Society
<b>Task Groups</b>	
LE Anderson	Member, World Health Organization Working Group on Health Protection for Nonionizing Radiation
	Member, International Conference on High-Voltage Electric Systems Working Group 36.06 on EMF and Health
LA Braby	Committee on Interagency Radiation Research & Policy Coordination (CIRRPC) Task Group, charged to assess research needs related to the biological effectiveness of neutron radiation
AL Brooks	Member and Past Chairman, DOE/OHER Task Group on Cellular and Molecular Biology
	Co-Chairman, Task Group 11, Liver Carcinogenesis, NCRP Committee 57
	Member, ICRP Task Group on Standard Man; responsible for information on liver
FJ Brockman	Bioremediation Technical Support Group, Savannah River Integrated Demonstration, DOE
FT Cross	Member, ICRP Task Group on Respiratory Tract Models
	Member, DOE/CEC Radon Risk Strategy Task Group
	Member, DOE/OHER Radon Principal Scientist Task Group
	Member, ICRP Task Group on Internal Dosimetry
	Member, Two ICRP Subtask Groups on Inhalation Dose Coefficients
GE Dagle	Member, NCRP Scientific Committee 57, Task Group 9 on Risk Estimates for Cancer of the Respiratory Tract from Inhaled Radionuclides
	Chairman, DOE/OHER Interlaboratory Task Group on Biological Effects
DR Fisher	DOE Expert Group on Internal Dosimetry
GW Gee	Member, W-155, Western Regional Research on Field-Scale Flow and Transport

Who	What
<b>Task Groups (contd)</b>	
ES Gilbert	Member, NCRP Scientific Committee 57, Task Group 9 on Risk Estimates for Cancer of the Respiratory Tract from Inhaled Radionuclides
TR Ginn	Member, ASCE Water Resources Systems Committee
J Glissmeyer	Chairman, ANSI N13.1 Working Group, Sampling of Airborne Radioactive Materials in Nuclear Facilities
AC James	Corresponding Member, ICRP Task Group on Dose Calculations Member, DOE/CEC Working Party on Radon-Related Risk Recommendations
NS Laulainen	Member, ARM Aerosol Working Group Member, ARM Instrument Team
SA Rawson	DOE/OHER representative to DOE/Office of Technology Development (OTD) In Situ Remediation Integrated Program Core Planning Group
JD Saffer	Member, IEEE Standards Coordinating Committee 28, Subcommittee 4 Literature Review Group
RD Smith	American Chemical Society (ACS) Analytical Division Program Committee
WT Spaeth	Program Associate, U.S. Global Change Research Program
GM Stokes	National Resource Council's National Council on Science Education Standards and Assessments
CD Whiteman	Member, National Spray Model Advisory Committee, USFS Chairman, Meteorological Committee, National Spray Model Advisory Committee, USFS Member, Technical Advisory Committee, Brown Cloud II: The Denver Air Quality Modeling Study
<b>Workshops and Conferences</b>	
F Brockman	Invited speaker, Hanford Chemical Conference: Past Accomplishments and Future Activities, Richland, Washington
FT Cross	Invited Speaker, NRC Radon Program, Molecular and Cellular Radiobiology Workshop, August 1993, Washington, DC Invited Participant, Joint Meeting of the ICRP with all Committees, September 1993, Bournemouth, England
GE Dagle	Invited Participant, Joint DOE/EULEP Workshop on Lung Pathology, Paris, France, October 1992
RJ Douthart	Invited speaker, DOE Human Genome Workshop, Santa Fe, New Mexico, February 1993
JA Edmonds	Invited speaker, International Energy Agency (IEA) Carbon Dioxide Disposal Symposium, Oxford, England, March 1993

Who	What
<b>Workshops and Conferences (contd)</b>	
JA Edmonds (contd)	<p>Invited speaker, Intergovernmental Panel on Climate Change, Working Group Three, Montreal, Canada, May 1993</p> <p>Invited speaker, Sixth Annual Federal Forecasters Conference, Crystal City, Virginia, September 1993</p> <p>Invited speaker, Keynote presentation to the Office of Technology Assessment Workshop, Climate Treaties and Models, sponsored by the Office of Technology Assessment, Washington, DC, April 1993</p> <p>Invited speaker, Global Change Institute Conference on the Carbon Cycle, Snowmass, Colorado, July 1993</p> <p>Invited speaker, International Workshop in Integrative Assessment of Mitigation, Impacts and Adaptation to Climate Change, Laxenburg, Austria, June 1993</p> <p>Invited speaker, American Enterprise Institute Seminar on the Administration's National Action Plan to Reduce Greenhouse Gas Emissions, Washington, DC, November 1993</p> <p>Invited speaker, Johns Hopkins University, Baltimore, Maryland, November 1993</p> <p>Invited speaker, International Workshop on Costs, Impacts, and Possible Benefits of CO<sub>2</sub> Mitigation, Laxenburg, Austria, June 1993</p> <p>Invited speaker, IPCC Working Group One, Shepperton, England, December 1993</p>
JK Fredrickson	Invited Speaker, Gordon Conference on Applied and Environmental Microbiology, July 1993
GW Gee	Invited Speaker, AGU Symposium on Recharge, May 1994, Baltimore, Maryland
SJ Ghan	Invited Speaker, National Center for Atmospheric Research Summer Colloquium on Clouds and Climate, July 1993
ES Gilbert	<p>Invited Speaker, DOE/RERF Information Workshop, April 1993, Irvine, California</p> <p>Invited Speaker, Conference on Biological Effects of Low Level Exposures (BELLE) to Chemicals and Radiation, April 1993, Washington, DC</p> <p>Invited Participant, CDC Workshop on Dose Reconstruction for Epidemiological Uses, October 1993, Washington, DC</p> <p>Invited Speaker, Advanced Workshop on Occupational and Environmental Radiation Protection, Boston, Massachusetts, August 1994</p>
AC James	<p>Invited Speaker, 33rd Annual Congress of South African Association of Physicists in Medicine and Biology (SAAPMB), March 1993, Bloemfontein, South Africa</p> <p>Invited Speaker, International Workshop on Indoor Radon Remedial Action, June 27-July 2, 1993, Rimini, Italy</p> <p>Invited Speaker, Radiobiology of Inhaled Nuclides Symposium, November 1993, Richland, Washington</p> <p>Invited Speaker, Special Symposium of Lung Deposition and Clearance Mechanisms, March 1994, Frankfurt, Germany</p>

Who	What
<b>Workshops and Conferences (contd)</b>	
RF Jostes	Invited Speaker, Workshop on Single-Cell Gel Techniques, Sixth International Congress on Environmental Mutagens, February 1993, Melbourne, Australia
RL Ornstein	Eighth Conversation: Biomolecular Stereodynamics, Albany, New York, June 1993 Midwest Cytochromes P450 Symposium, Purdue University, September 1993, West Lafayette, Indiana Hanford Technical Exchange Symposium, December 1993, Richland, Washington Battelle Bioremediation Workshop, January 1994, Tallahassee, Florida FASEB Meeting, April 1994, Anaheim, California World Congress on Computational Medicine, Public Health & Biotechnology, April 1994, Austin, Texas DOE Workshop on Lignin Biosynthesis & Biodegradation, May 1994, Asilomar, California Jerusalem Symposium in Quantum Chemistry & Biochemistry, May 1994, Jerusalem, Israel
SA Rawson	Invited Speaker, University of Virginia, Department of Environmental Sciences Colloquium, October 1993, Charlottesville, Virginia
LE Sever	Invited Speaker, Columbia Chapter Health Physics Society, Richland, Washington, October 1992 Invited Lecturer, Course on "Public Health Surveillance: Epidemiology and Public Policy," Departments of Epidemiology and Health Services, University of Washington School of Public Health and Community Medicine, Seattle, Washington, November 1992
W Shaw	Speaker, 21st Conference on Agricultural and Forest Meteorology, March 7-10, 1994, San Diego, California Speaker, Third International Symposium on Tropospheric Profiling: Needs and Technologies, August 30-September 2, 1994, Hamburg, Germany Speaker, Ninth Symposium on Meteorological Observations and Instrumentation, March 27-31, 1995, Charlotte, North Carolina
RD Smith	Plenary Lecturer, Fifth International Conference on Capillary Electrophoresis, January 31-February 3, 1993, Orlando, Florida Plenary Lecturer, Annual Meeting, Swedish Chemical Society, June 1993, Lund, Sweden Plenary Lecturer, ACS Summer Symposium on Analytical Biotechnology, June 1993, Boston, Massachusetts Plenary Lecturer, 10th Montraux Symposium on LC-MS and CE-MS, July 1993, Ithaca, New York Invited Speaker, ACS Symposium on Capillary Electrophoresis, August 1993, Chicago, Illinois

Who	What
<b>Workshops and Conferences (contd)</b>	
TS Tenforde	<p>Invited Speaker, National Research Council Air Force Studies Board Winter Meeting, January 1993, Washington, DC</p> <p>Invited Speaker, American Association for the Advancement of Science Annual Meeting, February 1993, Boston, Massachusetts</p> <p>Invited Speaker, Electricité de France Symposium, June 1993, Paris, France</p> <p>Invited Speaker and Session Chairman, IEEE Antennas and Propagation Society International Symposium, June 1993, Ann Arbor, Michigan</p> <p>Invited Speaker and Session Chairman, International Union of Radio Science 24th General Assembly, August 1993, Kyoto, Japan</p> <p>Invited Speaker and Rapporteur, International Symposium on Magnetic and Electromagnetic Fields, Kyushu University, September 1993, Fukuoka, Japan</p> <p>Invited Speaker, American Physical Society Spring Meeting, March 1994, Pittsburgh, Pennsylvania</p> <p>Invited Speaker and Session Chairman, NCRP Annual Meeting, April 1994, Arlington, Virginia</p> <p>Invited Speaker, U.S.-Japan Seminar on Electromagnetic Fields, June 1994, Sapporo, Japan</p> <p>Invited Speaker, Swedish National Institute of Occupational Health Symposium on Occupational Exposure Limits for Electromagnetic Fields, September 1994, Stockholm, Sweden</p>
RE Weller	Invited Speaker, Department of Comparative Medicine, University of Washington, April 1993, Seattle, Washington
CD Whiteman	<p>Invited Speaker, National Fire Weather Forecaster Training Course, February 23-March 4, 1993, Boise, Idaho</p> <p>Invited Presentation, Advances in Conceptual Models: ASCOT (1979-1995). Preprints, 7th Conference on Mountain Meteorology, Breckenridge, Colorado. American Meteorological Society, Boston, Massachusetts, July 17-21, 1995</p> <p>Invited Speaker, The Thermally Driven Winds, National Fire Weather Forecasters Training Course S-591, Fire Weather Book No. 1, Unit II-B, Boise, Idaho, March 7-16, 1995, National Weather Service</p>
RE Wildung	Board Division, Washington State University, Pullman, Washington
J Zachara	Invited Participant, National Science Foundation Workshop on Interdisciplinary Research in Environmental Sciences

## 7.5 OHER-Supported Publications 1993-1994

### Analytical Technology (KP-01)

### Measurement Science (KP-01-02)

#### 1993

Bruce, J. E., G. A. Anderson, S. A. Hofstadler, S. L. Van Orden, M. S. Sherman, A. L. Rockwood, and R. D. Smith. 1993. Selected-Ion Accumulation from an External Electrospray Ionization Source with a Fourier-Transform Ion Cyclotron Resonance Mass Spectrometer. *Rapid Commun. Mass Spectrom.* 7:914-919.

Bruce, J. E., G. A. Anderson, S. A. Hofstadler, B. E. Winger, and R. D. Smith. 1993. Time-Base Modulation for the Correction of Cyclotron Frequency Shifts Observed in Long-Lived Transients from Fourier-Transform Ion-Cyclotron-Resonance Mass Spectrometry of Electrosprayed Biopolymers. *Rapid Commun. Mass Spectrom.* 7:700-703.

Feller, D., E. D. Glendening, E. A. McCullough, Jr., and R. J. Miller. 1993. A Comparison of Unrestricted Hartree-Foch- and Restricted Open-Shell Hartree-Foch-Based Methods for Determining the Magnetic Hyperfine Parameters of NO ( $X^2\Pi$ ). *J. Chem. Phys.* 99(4):2829-2840.

Gale, D. C., and R. D. Smith. 1993. Small Volume and Low Flow-Rate Electrospray Ionization Mass Spectrometry of Aqueous Samples. *Rapid Commun. Mass Spectrom.* 7:1017-1021.

Goodlett, D. R., D. G. Camp, II, C. C. Hardin, M. Corregan, and R. D. Smith. 1993. Direct Observation of a DNA Quadruplex by Electrospray Ionization-Mass Spectrometry. *Biol. Mass Spectrom.* 22:181-183.

Goodlett, D. R., J. H. Wahl, H. R. Udseth, and R. D. Smith. 1993. Reduced Elution Speed Detection for Capillary Electrophoresis/Mass Spectrometry. *J. Microcol. Sep.* 5:57-62.

Hofstadler, S. A., J. H. Wahl, J. E. Bruce, and R. D. Smith. 1993. On-Line Capillary Electrophoresis with Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. *J. Am. Chem. Soc.* 115:6983-6984.

Light-Wahl, K. J., J. A. Loo, C. G. Edmonds, R. D. Smith, H. Ewa Witkowska, C.H.L. Shackleton, and C-S.C. Wu. 1993. Collisionally Activated Dissociation and Tandem Mass Spectrometry of Intact Hemoglobin  $\beta$ -Chain Variant Proteins with Electrospray Ionization. *Biol. Mass Spectrom.* 22:112-120.

Light-Wahl, K. J., B. E. Winger, and R. D. Smith. 1993. Observation of the Multimeric Forms of Concanavalin A by Electrospray Ionization Mass Spectrometry. *J. Am. Chem. Soc.* 115:5869-5870.

Light-Wahl, K. J., D. L. Springer, B. E. Winger, C. G. Edmonds, D. G. Camp, II, B. D. Thrall, and R. D. Smith. 1993. Observation of a Small Oligonucleotide Duplex by Electrospray Ionization Mass Spectrometry. *J. Am. Chem. Soc.* 115:803-804.

Loo, J. A., C. G. Edmonds, and R. D. Smith. 1993. Tandem Mass Spectrometry of Very Large Molecules. II. Dissociation of Multiply Charged Proline-Containing Proteins from Electrospray Ionization. *Anal. Chem.* 65:425-438.

Murphy, J. E., B. A. Bushaw, and R. J. Miller. 1993. Doppler-Free Two-Photon Fluorescence Excitation Spectroscopy of the  $A < -X(1,0)$  Band of Nitric Oxide: Fine Structure Parameter for the  $(3s\sigma)A^2\Sigma^+(v=1)$  Rydberg State of  $^{14}\text{N}^{16}\text{O}$ . *J. Mol. Spectrosc.* 159:217-229.

Ogorzalek Loo, R. R., D. R. Goodlett, R. D. Smith, and J. A. Loo. 1993. Observation of a Noncovalent Ribonuclease S-Protein/S-Peptide Complex by Electrospray Ionization Mass Spectrometry. *J. Am. Chem. Soc.* 115:4391-4392.

Pfund, D. M., J. L. Fulton, and R. D. Smith. 1993. Aggregation of Methanol in Supercritical Fluids. A Molecular Dynamics Study. In: *Supercritical Fluid Engineering Science: Fundamentals and Applications*, E. Kiran and J. F. Brennecke, eds., pp. 158-174. Proceedings of the ACS Symposium Series, November 17-22, 1991. American Chemical Society, Washington, D.C.

Smith, R. D., J. H. Wahl, D. R. Goodlett, and S. A. Hofstadler. 1993. Capillary Electrophoresis/Mass Spectrometry. *Anal. Chem.* 65:574A-584A.

Smith, R. D., and H. R. Udseth. 1993. Mass Spectrometric Detection for Capillary Electrophoresis. In: *Capillary Electrophoresis*, N. A. Guzman, ed., Chapter 6, pp. 525-567. Marcel Dekker, Inc., New York, New York.

Smith, R. D., J. H. Wahl, K. J. Light-Wahl, and B. E. Winger. 1993. New Developments in Microscale Separations and Mass Spectrometry for Biomonitoring: Capillary Electrophoresis and Electrospray Ionization Mass Spectrometry. *J. Toxicol. Environ. Health*, pp. 147-158.

Smith, R. D., and K. J. Light-Wahl. 1993. The Observation of Noncovalent Interactions in Solution by Electrospray Ionization Mass Spectrometry: Promise, Pitfalls, and Prognosis. *Biol. Mass. Spectrom.* 22:493-501.

Springer, D. L., R. J. Bull, S. C. Goheen, D. M. Sylvester, and C. G. Edmonds. 1993. Electrospray Ionization Mass Spectrometric Characterization of Acrylamide Adducts to Hemoglobin. In: *The Laboratory and Epidemiology: The Development and Application of Biomarkers to the Study of Human Health Effects*, L. E. Sever, ed., Proceedings of the 31st Hanford Symposium on Health and the Environment, October 19-23, 1992, Richland, Washington. *J. Toxicol. Environ. Health*, pp. 161-176.

Wahl, J. H., D. R. Goodlett, H. R. Udseth, and R. D. Smith. 1993. Use of Small-diameter Capillaries for Increasing Peptide and Protein Detection Sensitivity in Capillary Electrophoresis-Mass Spectrometry. *Electrophoresis* 14:448-457.

Winger, B. E., S. A. Hofstadler, J. E. Bruce, H. R. Udseth, and R. D. Smith. 1993. High-Resolution Accurate Mass Measurements of Biomolecules Using a New Electrospray Ionization Ion Cyclotron Resonance Mass Spectrometer. *J. Am. Soc. Mass. Spectrom.* 4:566-577.

Winger, B. E., K. J. Light-Wahl, R. R. Ogorzalek Loo, H. R. Udseth, and R. D. Smith. 1993. Observation and Implications of High Mass-to-Charge Ratio Ions from Electrospray Ionization Mass Spectrometry. *J. Am. Soc. Mass. Spectrom.* 4:536-545.

## 1994

Bakhtiar, R., Q. Wu, S. A. Hofstadler, and R. D. Smith. 1994. Charge State Specific Facile Gas-Phase Cleavage of Aspartyl 75-Methionine 76 Peptide Bond in the  $\alpha$ -Chain of Human Apohemoglobin Probed by Electrospray Ionization Mass Spectrometry. *Biomed. Mass Spectrom.* 23:707-710.

Bruce, J. E., S. A. Hofstadler, B. E. Winger, and R. D. Smith. 1994. Characterization of Ribonuclease B Heterogeneity and the Identification and Removal of Phosphate Adducts by High Resolution Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. *Intern. J. Mass Spectrum Ion Proc.* 132:97-107.

Bruce, J. E., X. Cheng, R. Bakhtiar, Q. Wu, S. A. Hofstadler, G. A. Anderson, and R. D. Smith. 1994. Trapping, Detection, and Mass Measurement of Individual Ions in a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. *J. Amer. Chem. Soc.* 116:7839-7847.

Gale, D. C., D. R. Goodlett, K. J. Light-Wahl, and R. D. Smith. 1994. Observation of Duplex DNA-Drug Noncovalent Complexes by Electrospray Ionization Mass Spectrometry. *J. Amer. Chem. Soc.* 116:6027-6028.

Goodlett, D. R., R. R. Ogorzalek Loo, J. A. Loo, J. H. Wahl, H. R. Udseth, and R. D. Smith. 1994. A Study of the Thermal Denaturation of Ribonuclease S by Electrospray Ionization-Mass Spectrometry. *J. Am. Soc. Mass Spectrom.* 5:614-622.

Hofstadler, S. A., J. E. Bruce, A. L. Rockwood, G. A. Anderson, B. E. Winger, and R. D. Smith. 1994. Isotopic Beat Patterns in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: Implications for High Resolution Mass Measurements of Large Biopolymers. *Intern. J. Mass Spectrom. Ion Proc.* 132:109-127.

Hofstadler, S. A., J. H. Wahl, R. Bakhtiar, G. A. Anderson, J. E. Bruce, and R. D. Smith. 1994. Capillary Electrophoresis Fourier Transform Ion Cyclotron Resonance Mass Spectrometry with Sustained Off-Resonance Irradiation for the Characterization of Protein and Peptide Mixtures. *J. Amer. Soc. Mass Spectrom.* 5:894-899.

Light-Wahl, K. J., B. L. Schwartz, and R. D. Smith. 1994. Observation of the Noncovalent Quaternary Associations of Proteins by Electrospray Ionization Mass Spectrometry. *J. Amer. Chem. Soc.* 116:5271-5278.

Loo, J. A., P. Hu, and R. D. Smith. 1994. Interaction of Angiotensin Peptides and Zinc Metal Ions Probed by Electrospray Ionization Mass Spectrometry. *J. Amer. Soc. Mass Spectrom.* 5:959-965.

Loo, R. R., B. E. Winger, and R. D. Smith. 1994. Proton Transfer Reactions of Multiple Charged Proteins in a High  $m/z$  Quadrupole Mass Spectrometer. *J. Amer. Soc. Mass Spectrom.* 94:1064-1071.

Ogorzalek Loo, R. R., and R. D. Smith. 1994. Investigation of the Gas Phase Structure of Electro sprayed Proteins Using Ion-Molecule Reactions. *J. Amer. Soc. Mass Spectrom.* 5:207-220.

Ogorzalek Loo, R. R., and R. D. Smith. 1994. Proton Transfer Reactions of Multiply Charged Peptide and Protein Cations and Anions. *J. Mass Spectrom.* 5:1064-1071.



Ogorzalek Loo, R. R., B. E. Winger, and R. D. Smith. 1994. Proton Transfer Reactions of Multiply Charged Proteins in a High Mass-to-Charge Ratio Quadrupole Mass Spectrometer. *J. Amer. Soc. Mass Spectrom.* 5:1064-1071.

Schwartz, B. L., K. J. Light-Wahl, and R. D. Smith. 1994. Observation of Noncovalent Complexes to the Avidin Tetramer by Electrospray Ionization Mass Spectrometry. *J. Am. Soc. Mass Spectrom.* 5:201-204.

Smith, R. D., X. Cheng, J. E. Bruce, S. A. Hofstadler, and G. A. Anderson. 1994. Trapping, Detection and Reaction of Very Large Single Molecular Ions by Mass Spectrometry. *Nature* 369:137-139.

Wahl, J. H., and R. D. Smith. 1994. Comparison of Buffer Systems and Interface Designs for Capillary Electrophoresis-Mass Spectrometry. *J. Cap. Electrophor.* 1:62-71.

Wahl, J. H., D. C. Gale, and R. D. Smith. 1994. Sheathless Capillary Electrophoresis-Electrospray Ionization Mass Spectrometry Using 10  $\mu$ m I.D. Capillaries: Analysis of Tryptic Digests of Cytochrome c. *J. Chromatogr. A* 659:217-222.

## **Environmental Research (KP-02)**

### **Atmospheric Science (KP-02-01)**

#### **1993**

Allwine, K. J. 1993. Atmospheric Dispersion and Tracer Ventilation in a Deep Mountain Valley. *J. Appl. Meteorol.* 32(6):1017-1037.

Allwine, K. J. 1993. PGEMS—An Atmospheric Dispersion Model for Emergency Response. *Preprints, Environmental Transport and Dosimetry*, August 31-September 3, 1993, Charleston, South Carolina. American Nuclear Society, La Grange Park, Illinois.

Doran, J. C. 1993. An Overview of the ASCOT Program. In: *Proceedings of the Topical Meeting on Environmental Transport and Dosimetry*, September 1-3, 1993, Charleston, South Carolina, pp. 31-35. American Nuclear Society, La Grange Park, Illinois.

Easter, R. C. 1993. Two Modified Versions of Bott's Positive-Definite Numerical Advection Scheme. *Mon. Wea. Rev.* 121(1):297-304.

Elderkin, C. E. 1993. Recent ASCOT Experiments in Multilayered Flows. In: *Proceedings of the Topical Meeting on Environmental Transport and Dosimetry*, September 1-3, 1993, Charleston, South Carolina, pp. 36-39. American Nuclear Society, La Grange Park, Illinois.

Elderkin, C. E., and P. H. Gudiksen. 1993. Transport and Dispersion in Complex Terrain. *Radiat. Prot. Dosim.* 50(2-4):265-271.

Hubbe, J. M., and K. J. Allwine. 1993. Mesoscale Meteorological Measurements Characterizing Complex Flows. *Preprints, Environmental Transport and Dosimetry*, August 31-September 3, 1993, Charleston, South Carolina, pp. 47-51. American Nuclear Society, La Grange Park, Illinois.

Porch, W. M., and W. Shaw. 1993. Application of Optical Remote Sensing to the Study of Surface Fluxes Related to Cloud Formation. *Proceedings of the Symposium on Optical Remote Sensing of the Atmosphere*, pp. 110-114, March 8-12, 1993, Park City, Utah. Optical Society of America.

Stannard, D. I., W. P. Kustas, K. J. Allwine, and D. E. Anderson. 1993. Micrometeorological Data Collection. Chapter V in: *Hydrology Data Report Washita '92*, T. J. Jackson and F. R. Schiebe, eds. NAWQL Report No. 93-1, National Agricultural Water Quality Laboratory, U.S.D.A. Agricultural Research Service, Durante, Oklahoma.

Whiteman, C. D., and J. C. Doran. 1993. The Relationship Between Overlying Synoptic-Scale Flows and Winds Within a Valley. *J. Appl. Meteor.* 32(11):1669-1682.

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