LBL-26582

RECEIVED
LAWRENCE
BERKELEY LABORATORY

SEP 1 9 1989

LIBRARY AND
DOCUMENTS SECTION

Annual Report

FY 1988

Applied Science Division

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks.

April 1989

Lawrence Berkeley Laboratory
University of California, Berkeley

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

LBL-26582

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBL-26582

APPLIED SCIENCE DIVISION ANNUAL REPORT FY 1988

Elton J. Cairns

Director, Applied Science Division

Applied Science Division
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, California 94720

Prepared for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098

STATEMENT OF THE DIVISION DIRECTOR

The Applied Science Division (ASD) of Lawrence Berkeley Laboratory (LBL) had its origins in the early 1970's in response to national concerns over energy and the environment. The nation's attention to these issues has waxed and waned over the years; for example, the recent decline of oil prices has led to a diminished interest in energy conservation. However, there is no doubt that over the longer term, the nation must make more efficient use of energy and develop new energy sources—especially because oil imports are a large and growing fraction of the trade deficit. Concerns over the health, environmental, and global climate impacts of energy use are increasing. The nation's international industrial competitiveness (e.g., for energy-related products) is an ongoing issue. The Division views its role as being in the forefront of the research effort that will help the nation address these concerns.

In 1988 the Division continued work in its major research areas: **energy conversion and storage** (advanced batteries and fuel cells, solar and fossil fuel conversion, biotechnology, materials for energy applications); **environmental research** (atmospheric and biospheric effects of combustion, combustion processes, analytical chemistry, membrane bioenergetics); **building sciences** (advanced electrical lighting, windows, daylighting, and thermally driven heat pumps; building energy use measurement, computer simulation, and prediction; building data compilation and analysis; indoor air quality); and **policy analysis** (energy conservation by energy utilities, international energy demand, environmental policy analysis, appliance efficiency standards).

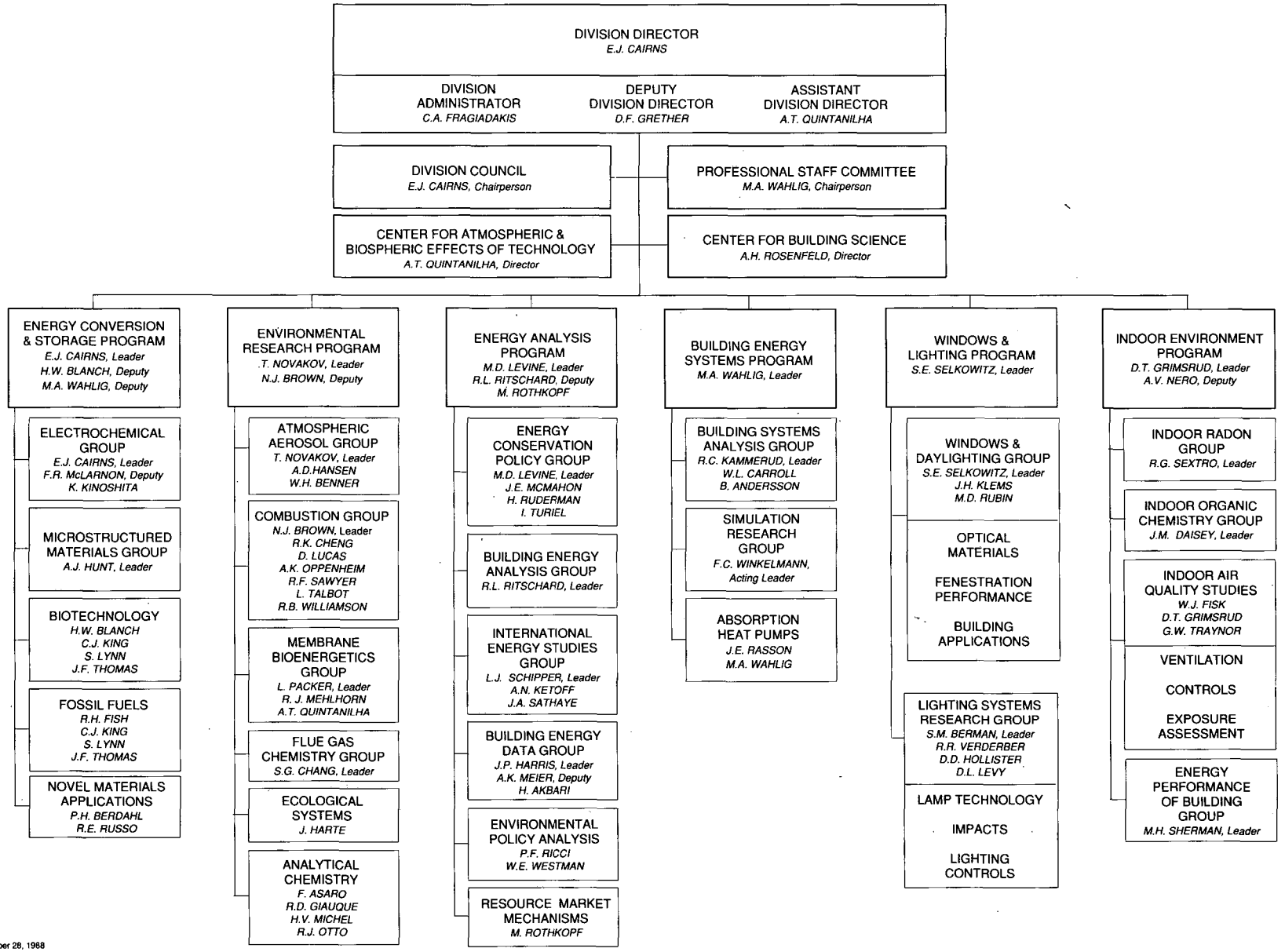
The Division also continued to develop new and expanded research areas. ASD has the lead in LBL's considerably enhanced research program on indoor radon. Working with the Materials and Chemical Sciences Division, a research program was established to investigate thin films of the recently discovered high-temperature superconductors for eventual applications in electrical power systems. In response to the growing concern over global warming from carbon dioxide and other "greenhouse" gases, ASD is increasing its activities in environmental research (e.g., cloud dynamics, impact on ecosystems) and analysis (e.g., potential for reducing emissions through energy efficiency, projected energy use in developing countries). Preliminary steps were made in a longer-term effort to develop advanced computer-based methods for designing buildings—methods which would readily permit incorporation of energy efficiency measures. Progress was made in establishing a research program on energy efficiency that would address the needs of the State of California.

Several ASD scientists received national recognition for their accomplishments. Samuel Berman was the first recipient of the Department of Energy's newly established Sadi Carnot Award in Energy Conservation. Berman received the award for his work (with Stephen Selkowitz) on low-emissivity coatings for windows and (with Rudy Verderber) on high-frequency solid-state ballasts for fluorescent lighting. Stephen Selkowitz and co-workers received a Federal Laboratory Consortium Award for Excellence in Technology Transfer for the development and transfer to industry of the WINDOW thermal analysis computer program. Selkowitz and his group were also selected to receive a citation from *Progressive Architecture* magazine for developing a Skylight Design Manual and software to help architects and engineers use skylights in a more energy-efficient manner. Anthony Nero was named as the 1989 recipient of the American Physical Society's Leo Szilard award for Physics in the Public Interest for his work on indoor air pollution (especially radon), nuclear proliferation, and reactor safety.

The Summary of Activities of the Applied Science Division addresses the above subjects in more detail, describes significant research accomplishments for 1988, and provides other information concerning the Division.

LAWRENCE BERKELEY LABORATORY

APPLIED SCIENCE DIVISION



WRB (TID) October 28, 1988

APPLIED SCIENCE DIVISION

Elton J. Cairns

Division Director

Cheryl Fragiadakis

Division Administrator

Donald F. Grether

Deputy Division Director

Alex Quintanilha

Assistant Division Director

DIVISION OFFICE STAFF

Anton Acker
Cynthia Bollinger
Camelia Griego
Mary Hart
Sandra Mocco
Maria Ossa
Rebecca Palmer
Rosa Rodriguez
Pat Ross
Lila Schwartz
Janet Smith
Angela Smothers
Zenaida Yuson

CONTENTS

Summary of Activities xiv

ENERGY CONVERSION AND STORAGE PROGRAM

Introduction 1-1

ELECTROCHEMICAL ENERGY STORAGE AND CONVERSION

Technology Base Research Project for Electrochemical Energy Storage
E.J. Cairns, K. Kinoshita, and F.R. McLarnon 1-2

Advanced Electrode Research
E.J. Cairns, F.R. McLarnon, T.C. Adler, M.J. Isaacson, K.G. Miller, S.A. Naftel, P. Ridgway, J. Rudnicki, R. Russo and J. Weaver 1-3

THERMOCHEMICAL ENERGY STORAGE AND CONVERSION

Direct Solar Thermal Conversion Processes
A. Hunt, I. Hodara, F. Miller, and J. Noring 1-7

Microstructured Materials
A. Hunt, F. Hibbler, and K. Lofftus 1-8

Light Scattering Studies
A. Hunt, K. Lofftus, A. Quintanilha, M. Quinby-Hunt, H. Salamon, R. Macy, and D. Shapiro 1-9

High-Temperature Superconducting Films: Electrical Characterization
P. Berdahl and L. Williams 1-10

High-Temperature Superconductors: Fundamentals and their Applications
P. Berdahl 1-11

Solid-State Radiative Heat Pump
P. Berdahl 1-11

COAL-RELATED RESEARCH

Processing of Condensate Waters from Coal Gasification
C.J. King, T. Grant, and L. Poole 1-13

Removal of H_2S from Coal-Derived Gases
S. Lynn, T. Colson, R. Hix, and C. Stevens 1-13

ENERGY-RELATED CHEMISTRY

Organometallic Synthesis and Catalysis Studies
R.H. Fish, H-S. Kim, J.E. Babin, R.D. Adams, R.H. Fong, J.B. Vincent, J.C. Huffman, G. Christou, Q. Li, M.A. Nanny, and D.N. Hendrikson 1-16

Energy-Related Organic Compounds (EROC): A Microcomputer Information Database of Potential Pollutants
C.G. Daughton and J.F. Thomas 1-17

Studies of Animal Cell Cultures in Hollow-Fiber Reactors
E. Fernandez, A Mancuso, D. Clark, and H. Blanch 1-18

Separations by Reversible Chemical Association
C.J. King, A.S. Kertes, J. Tamada, D. Arenson, A. Garcia, L. Poole, J. Starr, W. Rixey, and M. Ng 1-19

Ultrasensitive Laser Spectroscopy
R.E. Russo, J.D. Spear, and R.J. Silva 1-20

Pulsed Laser Ablation for Thin-Film High-Temperature Superconductors
R.E. Russo and B. Olson *1-21*

ENVIRONMENTAL RESEARCH PROGRAM

Introduction 2-1

ATMOSPHERIC AEROSOLS

Cloud Nucleation Characteristics of Smokes from Different Fuels
A.D.A. Hansen and T. Novakov 2-2

Acceleration of Submicron-Sized Particles
W.H. Benner and R. Otto 2-2

NO_2 and SO_2 Reactions on Cold Surfaces
W.H. Benner, A. Mizrahi, and T. Novakov 2-3

Sulfate Formation by Reaction of SO_2 with NH_3
W.H. Benner, B. Ogorevc, and T. Novakov 2-3

FLUE GAS CHEMISTRY

Removal of NO from Flue Gas by Tetrasulfophthalocyanine Complexes of Iron (II) and Cobalt (II)
D.K. Liu, G. Stevens, and S.G. Chang 2-5

Removal of Nitrogen and Sulfur Oxides from Flue Gas Using Aqueous Emulsions of Yellow Phosphorus and Alkali
D.K. Liu and S.G. Chang 2-5

A Study of the Hydrolysis of Disulfate Ion
D.X. Shen, D. Littlejohn, and S.G. Chang 2-6

The Chemistry of Bisulfite Ion in Aqueous Solution
D. Littlejohn, A. Li, and S.G. Chang 2-6

COMBUSTION

Controlled Combustion
D.W. Faris, K. Hom, J.A. Maxson, A.K. Oppenheim, and H.E. Stewart 2-8

Combustion Chemistry
N.J. Brown and R.J. Martin 2-9

Combustion Fluid Mechanics
R.K. Cheng, I.G. Shepherd, and L. Talbot 2-10

Smoke Emission Measurements from Medium-Scale Experiments
R.B. Williamson, R. Dod, C.M. Fleischman, N. Brown, and T. Novakov 2-11

MEMBRANE BIOENERGETICS

Photochemical Conversion of Solar Energy by Microbial Systems
L. Packer, R.J. Mehlhorn, I.V. Fry, J.J. Maguire, S. Spath, G. Khomutov, W. Nitchmann, E. Hrabeta-Robinson, M. Huflejt, J. Hrabeta, C. Reveron, J. Park, and K. Kondo 2-13

Detection and Prevention of Biological Free Radical Damage
R.J. Mehlhorn, J.J. Maguire, K. Moore, B. Stone, J. O'Neil-Gonzalez, L. Packer, and H. Rapoport 2-14

ANALYTICAL CHEMISTRY

Impacts of Large Extraterrestrial Bodies and Mass Extinctions
F. Asaro, H.V. Michel, L.W. Alvarez, W. Alvarez, and A. Montanari 2-16

A Study of the Relation Between Volcanism in the Weddell Sea about 65 Million Years Ago and the Cretaceous-Tertiary Bolide Impact
H.V. Michael, F. Asaro, W. Alvarez, and and L.W. Alvarez 2-16

Sources of Quartzite in Ancient Egyptian Sculptures
F.H. Stross, R.L. Hay, F. Asaro, H.R. Bowman, and H.V. Michel 2-17

Possible Worldwide Middle Miocene Iridium Anomaly and Its Relation to Periodicity of Impacts and Extinctions
F. Asaro, W. Alvarez, H.V. Michel, L.W. Alvarez, M.H. Anders, A. Montanari, and J.P. Kennett 2-18

ENERGY ANALYSIS PROGRAM

Introduction 3-1

BUILDING ENERGY ANALYSIS

Utility Accounting in Public Housing
R. Ritschard, K. Greely 3-2

Energy Management Practices in Public Housing
E. Vine 3-2

Energy Requirements for Multifamily Buildings
R. Ritschard, Y.J. Huang 3-3

A Comparison of Central vs. Individual HVAC and DHW Systems in Multifamily Buildings
S. Byrne 3-3

Analysis of Energy Performance of Unbalanced Single-Pipe Steam Heating Systems in Multifamily Buildings
Y.J. Huang, R. Ritschard 3-4

BUILDING ENERGY DATA

Estimating Nationwide Conservation Potential from Measured Data
K.M. Greely, A. Meier, C. Goldman, J. Harris 3-5

Least-Cost Utility Planning
F. Krause, J.P. Harris, M. Levine, A.H. Rosenfeld 3-6

Rated vs. Measured Energy Use of Refrigerators
A. Meier, K. Heinemeier 3-7

Experience with Energy Efficiency Programs for New Buildings
E. Vine, J. Harris 3-8

Analysis of Commercial Electric End-Use Data
H. Akbari, I. Turiel, J. Eto, L. Rainer 3-9

Development of a Simplified Tool to Calculate Commercial Sector EUIs
I. Turiel, B. Lebot 3-9

Comparative Assessment of the DSM Plans of Four New York Utilities
C. Goldman, E. Kahn 3-10

Energy Use and Efficiency of Electronic Office Equipment
J. Harris 3-11

EMCS for Utility/Customer Interface
H. Akbari, M. Goralka, K. Heinemeier 3-12

Field Measurement of Heat Island Data
H. Akbari, L. Rainer, H. Taha 3-13

Analysis of Residential End-Use Load Shapes
H. Ruderman, J.H. Eto, K.E. Heinemeier, A. Golan, D. Wood 3-14

ENERGY CONSERVATION POLICY

Analysis of Federal Appliance Efficiency Standards
H. Ruderman, P. Chan, P. Cunliffe, A. Heydari, J. Hobart, J. Koomey, B. Lebot, M. Levine, J. McMahon, T. Springer, S. Stoft, I. Turiel, D. Wood 3-15

Engineering Analyses of Appliance Efficiency Improvements
I. Turiel, A. Heydari, B. Lebot 3-16

Assessment of Impacts of Appliance Standards on Manufacturers
S. Stoft, P. Cunliffe, J. Hobart 3-17

Residential Energy Demand Forecasting
J. McMahon, P. Chan 3-18

The Regional Energy and Economic Impacts of Appliance Efficiency Standards
J. Eto, J. McMahon, J.G. Koomey, P. Chan, M. Levine 3-18

Research and Policy Studies to Promote Building Energy Efficiency in Southeast Asia
M. Levine, J. Deringer, J. Busch, Y.J. Huang, H. Akbari, K. Olson 3-19

ENVIRONMENTAL POLICY ANALYSIS

Global Biodiversity: Habitat Change and Species Extinctions
W. Westman 3-22

Effects of Climate Change on Vegetation in California and Baja California
W. Westman 3-23

INTERNATIONAL ENERGY STUDIES

Contribution of LDC Energy Use to the Global Climate Problem
J. Sathaye, A. Ketoff, L.ipper, S. Lele 3-24

European Electric Power Generation: The Role of Oil
D. Hawk, L. Schipper 3-25

Residential Energy Conservation Policy and Programs in Six OECD Countries
D. Wilson, L. Schipper, S. Tyler, S. Bartlett 3-26

Home Electricity Use in the OECD Countries: Recent Changes
L. Schipper, D. Hawk, A. Ketoff, N. Hirt 3-27

Electricity in the LDCs: Trends in Supply and Use Since 1970
S. Meyers, J. Sathaye 3-28

Production, Consumption, and Trade of Natural Gas: Western Europe and the Developing Countries
J. Sathaye, A. Ketoff, G. Pireddu 3-29

Energy Markets and Energy Demand: China and the U.S.
J. Sathaye, L. Schipper, M. Levine 3-30

RESOURCE MARKET MECHANISMS

Competition in Electricity Generation
E. Kahn 3-31

BUILDING ENERGY SYSTEMS PROGRAM

Introduction 4-1

Building Systems Analysis
R.C. Kammerud, B. Andersson, J. Birdsall, W.L. Carroll D. Dumortier, B. Hatfield, R.J. Hitchcock, J. Eto, F. Winkelmann, E. Vine 4-2

Absorption Heat Pumps
M. Wahlig, J. Rasson, M. Warren 4-5

Simulation Research
F.C. Winkelmann, B.E. Birdsall, W.F. Buhl, K.L. Ellington, A.E. Erdem, J.M. Nataf, E.F. Sowell 4-6

WINDOWS AND LIGHTING PROGRAM

Introduction 5-1

Windows and Daylighting
S.E. Selkowitz, D. Arasteh, C. Benton, D.L. DiBartolomeo, R.L. Johnson, J.J. Kim, J.H. Klems, C.M. Lampert, K. Papamichael, M.D. Rubin, R. Sullivan, and G.M. Wilde 5-2

Lighting Systems Research
S.M. Berman, R.R. Verderber, R.D. Clear, D. Crawford, D.D. Hollister, D.J. Levy, O.C. Morse, F.M. Rubinstein, M.J. Siminovitch, G.J. Ward, and R. Whiteman 5-11

INDOOR ENVIRONMENT PROGRAM

Introduction 6-1

INDOOR RADON

Evaluation of Several Techniques to Reduce Radon: Preliminary Results from Fourteen Houses
B.H. Turk, J. Harrison, R.G. Sextro, L.M. Hubbard, K.J. Gadsby, T.G. Matthews, C.S. Dudney, and D.C. Sanchez 6-2

Intensive Radon Mitigation Research: Lessons Learned
B.H. Turk, R.J. Prill, R.G. Sextro, and J. Harrison 6-2

Monitoring and Evaluation of Radon Mitigation Systems Over a Two-Year Period
R.J. Prill 6-3

Appraisal of the U.S. Data on Indoor Radon Concentrations
A.V. Nero, K.L. Revzan, and R.G. Sextro 6-3

Parametric Modelling of Temporal Variations in Radon Concentrations in Homes
K.L. Revzan, B.H. Turk, J. Harrison, A.V. Nero, and R.G. Sextro 6-5

Technique for Measuring the Indoor ^{222}Rn Source Potential of Soil
W.W. Nazaroff and R.G. Sextro 6-6

Mapping Surficial Radium Content as a Partial Indicator of Radon Concentrations in U.S. Houses
K.L. Revzan, A.V. Nero, and R.G. Sextro 6-7

INDOOR ORGANIC CHEMISTRY

Indoor Atmospheric Chemistry: Interactions of Radon with other Gaseous Pollutants
J.M. Daisey, R. Sextro, A.T. Hodgson, N. Brown, and D. Lucas 6-9

Initial Efficiencies of Air Cleaners for the Removal of Nitrogen Dioxide and Volatile Organic Compounds
J.M. Daisey and A.T. Hodgson 6-9

Volatile Organic Compounds in Large Buildings
J.M. Daisey and A.T. Hodgson 6-10

Development of a Sampling and Analysis Method for Polycyclic Aromatic Compounds in Indoor Air
J.M. Daisey, L.A. Gundel, A.T. Hodgson, and F.J. Offermann 6-11

The Role of Heterogeneous Reactions of NO_2 in Indoor Air
J.M. Daisey and L.A. Gundel 6-11

Transport of Volatile Organic Compounds from Soil into a Residential Basement
A.T. Hodgson, K. Garbesi, R.G. Sextro, and J.M. Daisey 6-12

INDOOR AIR QUALITY AND CONTROLS

The Indoor Environment of Commercial Buildings
D.T. Grimsrud, J.T. Brown, W.J. Fisk, and J.R. Girman 6-12

Pacific Northwest Existing Home Indoor Air Quality Survey and Weatherization Sensitivity Study
B.H. Turk, D.T. Grimsrud, J. Harrison, R. J. Prill, and K.L. Revzan 6-13

Commercial Building Ventilation Measurements Using Multiple Tracer Gases
W.J. Fisk, R.J. Prill, and O. Seppanen 6-14

INDOOR EXPOSURE ASSESSMENT

Indoor Exposure Assessment
G.W. Traynor, A.V. Nero, S.R. Brown, M.A. Apte, and B.V. Smith 6-15

ENERGY PERFORMANCE OF BUILDINGS

Energy Performance of Buildings
M.H. Sherman, R.C. Diamond, D.J. Dickerhoff, H.E. Feustel, M.K. Herrlin, A. Kovach, M.P. Modera, B.V. Smith, C. Stoker, and Y. Utsumi 6-17

PUBLICATIONS LIST 6-23

SUMMARY OF ACTIVITIES

The 1988 fiscal year (FY88) was a time of accomplishment and change for the Division. In the following sections are described several selected scientific accomplishments, major changes to the research directions of the Division, national recognition achieved by Division scientists, and other notable activities and events.

Recent Scientific Accomplishments

As an initial step in investigating indoor atmospheric chemistry, Joan Daisey and co-workers have obtained results on the **reaction of nitrogen dioxide on the surfaces of indoor materials**. While "outdoor" atmospheric chemistry is a well-developed field, the "indoor" counterpart is at an embryonic stage. Surface reactions are likely to be much more important in indoor than outdoor atmospheric chemistry because of the higher surface-to-volume ratio indoors and the dominance of photochemistry outdoors. Surface reactions of NO_2 (a combustion product) on indoor materials were investigated in a bench-top experiment. The materials investigated (polyurethane foam, nylon and wool carpet) removed NO_2 and produced some NO. Airborne nitrous acid (HNO_2) was produced by foam (18 ppb) and by wool carpet (4 ppb) for initial NO_2 concentrations of about 400 ppb. For comparison, outdoor concentrations of HNO_2 in highly polluted urban air range from 2 to 8 ppb. HNO_2 can initiate other indoor reactions which may lead to the formation of irritants and mutagens. Exposure to HNO_2 may also cause *in vivo* reactions in the lung to form carcinogenic N-nitrosamines.

Jayant Sathaye and co-workers developed **LDC scenarios for the Environmental Protection Agency (EPA) Report to Congress**. EPA was called upon to report to Congress on (1) environmental effects of global climate change and (2) options to both limit and adapt to global warming. LBL's role was to hold a workshop (May, 1988) on *Energy Efficiency and Structural Change: Implications for the Greenhouse Problem* and to develop scenarios of future energy use (and the resulting CO_2 emissions) for the Less Developed Countries (LDC's). Results obtained in the LBL study show that if present trends continue, energy demand in the LDC's will approach that of the developed countries by 2010. Analyses of these trends indicates that the LDC share will be dominant by 2025. The study also indicates that policies to reduce energy demand will have a greater impact on the developed countries than on the LDC's. The LBL results are a major component of the EPA analysis of global trends in CO_2 emissions and predictions of the resultant global warming. At the end of FY88, the EPA report was approaching final form.

Donald Levy has developed **higher-pressure surface wave medium-intensity discharge (MID) lamps**. In the *surface wave* approach, RF (radio frequency) power is used to ignite the plasma preferentially near the surface of the lamp enclosure, permitting higher efficiency and electrodeless operation. A major ongoing effort involves applying the surface wave concept to replacing the standard low-pressure fluorescent lamp (power loading of 1 watt/inch). Recent research has extended the surface wave approach to a higher-pressure, medium-intensity discharge (MID) lamp (10 watts/inch). The surface wave MID is a candidate for certain applications for which the present high-intensity discharge (HID) lamp (100 watts/inch) is not suitable. Available commercial HID's are quite efficacious and can be focused (as fluorescents cannot), e.g., for illumination of merchandise displays; however, the long ignition periods of these HID's (10-15 minutes) limits their applications. The surface wave MID's have been demonstrated to have instant restrike capability with zero reflected power. The combination of focusability and instant restrike make the surface wave MID an attractive high-efficiency candidate for replacing the assortment of low-efficiency incandescent lamps used for display purposes.

A **field validation of the WINDOW calculational approach** was accomplished under the leadership of Joseph Klems using the MoWiTT (Mobile Window Thermal Test) facility. Developed at LBL, MoWiTT is essentially a heavily instrumented calorimeter mounted in a mobile trailer and used to characterize the performance of full-scale window systems under actual weather conditions. WINDOW, also developed at LBL, is widely used by industry to predict the performance of fenestration systems (see the *Recognition* section later in this Summary). The MoWiTT results showed that the measured U-values for conventional single- and double-glazed windows accurately match those calculated *ab initio* using WINDOW when the calculation includes the actual exterior conditions and an approximation of the thermal bridging effects of the frame and spacer. Further, for windows with frames that have comparable thermal resistance to the central glazing, the WINDOW and MoWiTT results are consistent with commercial test laboratory measurements when differences between laboratory and field exterior conditions are taken into account. This result may pave the way for the formulation and adoption of window standards, which have been delayed for over a decade because of a lack of demonstrated consistency among the three methods (field, laboratory, calculation). For windows with frames that are significantly more conductive than the glazing, the laboratory measurements did not agree well with MoWiTT and WINDOW, raising the possibility of a

systematic error in the commercial test method for such windows. This issue will be investigated in detail in an upcoming project.

Henry Benner and Tihomir Novakov have obtained preliminary results on **scavenging and chemical transformation of NO_2 and SO_2 on cold surfaces by condensing water vapor**. Many environmentally important processes, including the formation of liquid water drops and ice particles in clouds, involve condensation of water vapor to the liquid or solid phase. The interactions of trace gas species with condensed water phases are of importance in understanding stratospheric ozone depletion and acid rain. Other investigators have studied the interactions of gaseous species with, for example, a pre-existing ice surface. The approach taken by Benner and Novakov is to investigate the physical and chemical interactions that occur as water is condensing on a surface; specifically, the scavenging and chemical transformation of NO_2 and SO_2 on low-temperature surfaces in the presence and absence of water vapor condensation. The results showed (1) a large fraction of NO_2 is scavenged when water vapor is initially present in the system; (2) SO_2 scavenging is about two orders of magnitude less efficient than of NO_2 under similar experimental conditions; (3) the scavenging of NO_2 is independent of the presence of SO_2; and (4) detectable sulfate concentrations observed only when NO_2 was present. The implications of these and other results for the issues of acidification of terrestrial surfaces and denitrification of the polar stratosphere will be addressed in future work.

Research Trends

As a result of work at LBL and elsewhere, **indoor radon** has received national attention as a health risk in single family residences. In response, DOE's Office of Health and Environmental Research (OHER) increased its support for radon-related research in FY87 and again in FY88. In FY87, the Division had received a funding increase for its ongoing radon characterization research, which includes soil transport, entry mechanisms, and indoor levels of radon. In FY88, support was received for two new projects. The first, a joint ASD/Earth Sciences Division (ESD) effort compares radon availability and migration through various soils by means of small instrumented structures with controlled leakage characteristics. A mathematical modeling effort will complement the experimental work. The project is being led by Richard Sextro of ASD, and Harold Wollenberg and T.N. Narasimhan of ESD. The second project, led by Joan Daisey, investigates the interactions of radon with other gaseous pollutants. Such interactions are one aspect of the more general topic of indoor atmospheric chemistry (see also *reactions of nitrogen dioxide on the surfaces of indoor materials under Recent Scientific Accomplishments*).

Research is underway in many institutions on the **new high-temperature (high t_c) superconductors**. ASD was the LBL participant in an assessment of applications that would conserve energy or (more broadly) improve energy productivity. The study, completed during FY88, was jointly conducted by DOE's Office of Conservation and the Electric Power Research Institute (EPRI). LBL's main contribution, carried out by Paul Berdahl, was to delineate the basic physical processes and to examine novel concepts. In early 1988, DOE's Office of Energy Storage & Distribution (OESD) initiated a Superconducting Technology for Electric Power Systems (STEPS) program. Under the leadership of Norman Phillips of the Materials and Chemical Sciences Division (MCSD), LBL submitted a multidivision proposal with three components: (1) thin-film production (ASD); (2) development of tape conductors (MCSD); and (3) magnet design (Accelerator & Fusion Research Division). OESD approved the work on thin films but held the conductor and magnet research in abeyance. Based on expertise in developing thin films for windows, Michael Rubin is using magnetron sputtering to deposit films on a variety of substrates. Based on a background in laser-material interactions, Richard Russo is producing as-deposited superconducting films using the laser ablation method. Arlon Hunt, with expertise on the sol-gel process for aerogels and ceramics, is initially developing chemical precursors for making films using the sol-gel process. Berdahl, with a background in superconductor theory and solid-state materials and devices, is developing a system for providing state-of-the-art characterization for the other investigators. At the end of FY88, efforts were underway towards developing collaborations with industrial partners.

In response to the growing concern over **global climate change** from CO_2 and other "greenhouse" gases, the Division is increasing its activities in both the environmental research and analysis areas. These activities are becoming a major focus of the Division's Center for Atmospheric and Biospheric Effects of Technology (CABET), headed by Alexandre Quintanilha. Although the CO_2 buildup is indisputable, much debate exists over the consequences as predicted by global climate models. The treatment of clouds is a major source of uncertainty in these models. Tihomir Novakov and co-workers have developed a unique laboratory facility: a cloud chamber which can be used to investigate cloud formation, chemistry, and optical properties. This capability will be the basis for proposals to DOE and NASA. In contrast to the situation for CO_2, the source of nitrous oxide (N_2O, another greenhouse gas) is not well understood. Nancy Brown is proposing to the EPA to study N_2O chemistry in the combustion process, a potential source for the gas. The CO_2 buildup and any resulting climate change (e.g., temperature increase, altered precipitation patterns) will almost certainly affect natural and agricultural ecosystems. Walter Westman and collaborators are proposing to DOE to study the effect on western conifer forests through both modeling and field experiments.

Turning to the analysis area, mention has already been made of the Division's role in EPA's reports to Congress on global climate change. (See *LDC Scenarios for the EPA Report to Congress* in the *Recent Scientific Accom-*

plishments section of this Summary.) In FY88, Congress appropriated funds (for FY89) to DOE's Office of Environmental Health & Safety (EH&S) to prepare reports on related issues. Mark Levine and others in the Energy Analysis Program are proposing to contribute to these reports by (1) delineating the potential for reductions of emissions through energy efficiency; (2) projecting future energy use in developing countries; (3) developing an inventory of data on greenhouse gas emissions; and (4) investigating alternatives to China's planned massive increase in the use of coal, among other topics. The University of California at Davis has proposed to EH&S that the University conduct workshops (and possibly an international meeting) that would help provide input to the reports to Congress. UCD asked LBL and Lawrence Livermore National Laboratory (LLNL) to assist in the planning process. The LBL participants are Mark Levine, Alexandre Quintanilha, and Martha Krebs, Associate Laboratory Director for Planning and Development.

Study of **summer urban heat islands** is a developing research area related in some respects to the global climate change issue. We have known for some time that urban areas tend to be several degrees warmer than surrounding rural areas because of higher rates of energy use and dark surfaces (roofs and roads) which absorb solar radiation. Higher temperatures lead to a greater use of air conditioning; this, of course, compounds the problem. Conversely, reducing the urban heat island effect would save energy and reduce urban air pollution because of reduced emissions. Light surfaces (e.g., white-washed buildings) and trees are well known to reduce urban temperatures. (Trees can shade individual houses and collectively cool the urban area through evapotranspiration.) However, to permit communities to embark on programs to revamp the urban landscape, quantitative information is needed, e.g., on expected temperature reduction, energy savings, and cost effectiveness of a given measure; choice of trees; and impact on water resources. Under the leadership of Arthur Rosenfeld and Hashem Akbari, the Division has undertaken some modest modeling and measurement projects which indicate the potential for reducing the urban heat island effect. A workshop planned for early 1989 will bring together experts on various aspects of the issue. Support will be sought from DOE and other agencies for a research effort that would yield the needed information.

Progress was made toward developing a longer-term research effort on **advanced computer-based building design**. The overall concept is to develop methods which readily permit incorporation of energy efficiency measures into the design and operation of buildings. The premise is that such recent technological developments as computer-aided design (CAD) systems with sophisticated graphics, expert systems, and computer-accessible mass storage will slowly replace the traditional design methods. An opportunity thus exists for energy conservation to be integrated into the new methods. The envisioned system would be built upon the buildings expertise at LBL and at other national laboratories and would become a vehicle for technology transfer of DOE's research products to the buildings industry. During FY88, the concept became an official Initiative of the Laboratory and as such is included in the LBL Institutional Plan for FY89-94. The Initiative received Exploratory R&D funds ("seed money") from the Laboratory for FY89 (with Stephen Selkowitz as the principal investigator) to support preliminary research and to develop contacts with the computer graphics industry. The concept has been presented to the DOE/Office of Buildings & Community Systems (OBCS) and may be included as an OBCS Initiative in the DOE Energy Conservation Multi-year Plan for FY91-95 (to be published in the Fall of 1989).

Recognition

Samuel Berman was named the first recipient of the Department of Energy's newly established **Sadi Carnot Award in Energy Conservation**. DOE annually presents the Enrico Fermi Award and the Ernest O. Lawrence Award, which date back to the days of the Atomic Energy Commission. However, these awards are intended for accomplishments associated with atomic energy (broadly interpreted) and in effect exclude achievements in non-nuclear energy technologies. Therefore, in 1988 DOE established a new award in each of three areas: conservation (Sadi Carnot award), renewables (John Ericsson award), and fossil energy (Homer H. Lowry award). Dr. Berman will receive the Carnot award at a ceremony in November at DOE Headquarters in Washington for his work (with Stephen Selkowitz) on low-emissivity coatings for windows and (with Rudy Verderber) on high-frequency solid-state ballasts for fluorescent lighting. Working with Donald Levy, Berman has developed the surface wave fluorescent lamp is which 40% more efficient than typical fluorescents. With Donald Jewett of the UC San Francisco medical center, Berman has made fundamental contributions to the understanding of the way the human eye reacts to different lighting conditions.

Stephen Selkowitz and co-workers in the Windows & Daylighting Group received a **Federal Laboratory Consortium Award for Excellence in Technology Transfer** for the development and transfer to industry of the WINDOW thermal analysis computer program. Originally developed as an in-house research tool, WINDOW represents an innovative approach to technology transfer. In 1986, the Group distributed a PC-compatible version, WINDOW 2.0, to about 100 major manufacturers of window products. Although the program was well received, resources were not available to distribute the program to smaller companies. Bostik Construction Products (a division of the Emhart Chemical Group) agreed to reproduce and distribute the diskette as a professional courtesy. The company used direct mail, the Bostik sales force, and trade shows to distribute the program to companies representing more than half the insulating glass industry sales. The Group will also receive (in early 1989) a **citation from** *Progressive Architecture* **magazine**. The citation, in the Applied Research category, is for the development of a

Skylight Design Manual and accompanying software to help architects and engineers use skylights in a more energy-efficient manner. The citation will be shared with Charles Eley and Associates, the architectural firm that worked with LBL to develop the manual under co-sponsorship of DOE and the American Architectural Manufacturing Association. Selkowitz's group had previously (1985) received a *Progressive Architecture* award for the Sky Simulator research facility.

Anthony Nero was named as the 1989 recipient of the **American Physical Society's Leo Szilard Award for Physics in the Public Interest** for his work on indoor air pollution (especially radon), nuclear proliferation, and reactor safety. Over the last ten years, Nero and his LBL colleagues did much of the work which led to the recognition of indoor radon as a major health hazard. Among other accomplishments, they showed that the major source of radon is the soil, that radon is drawn into buildings by pressure-driven flows, and that certain remedial measures can effectively reduce indoor radon levels. Nero and William Nazaroff co-edited the book *Radon and its Decay Products in Indoor Air,* published in 1988 and already considered a standard reference work on the subject. Nero will receive the Szilard award at a ceremony during the APS annual meeting in Baltimore in May. He is the second ASD scientist to receive the award; Arthur Rosenfeld was the recipient in 1986.

Other Notable Activities and Events

The Division's **Center for Building Science** (Arthur Rosenfeld, Director) continued to focus on establishing a research program on energy efficiency that would address the needs of the State of California. This effort, known as the California Institute for Energy Efficiency (CIEE), would coordinate research at LBL, the campuses of the University of California, and other California research institutions. Funding would be provided primarily by the California energy utilities; encouragement would be given by the California Energy Commission and California Public Utilities Commission; and the technology would be transferred back to the utilities for the ultimate benefit of California rate payers. During FY87, some early CIEE research projects were started; however, the administrative arrangements were somewhat ad hoc because CIEE was not yet an official organizational entity. An important milestone was reached in May, 1988, when the Office of the President of the University of California established CIEE as a provisional Organized Research Unit (ORU) of the University, administered by LBL. LBL Director David A. Shirley appointed Rosenfeld the acting Director of CIEE, which LBL designated a *Private Sector/Technology Transfer Initiative* and described in the LBL Institutional Plan for FY89-94.

Several additional steps remain before CIEE is functioning as planned: a mechanism will be established so that funding from the utilities will go to the University (acting on behalf of CIEE), and from there to LBL, UC campuses, and other research institutions; a high-level Research Board will be formed to set overall policy and directions; and technical panels will be created to aid in selecting research projects.

After more than a year of planning, a one-year **international workshop entitled Conjunction Of Multizone Infiltration Specialists (COMIS)** was convened at LBL in late FY88. The main organizers of the workshop are Max Sherman and Helmut Feustel of the Indoor Environment Program. Scientists from some nine countries will spend periods of time ranging from several months to the full year working at LBL to develop a detailed, user-friendly, multizone infiltration model that takes into account crack flow; heating, ventilating, and air conditioning (HVAC) systems; ventilation; and transport through large openings. Multigas tracer measurements and wind tunnel data will be used to validate the model. In addition, COMIS will produce documentation so that researchers throughout the world will be able to readily use the model.

Alex Quintanilha was appointed the Director of the **Center for Atmospheric and Biospheric Effects of Combustion** (CABEC) in FY87. During FY88, the Center was evaluated in light of developments over the past few years. Originally, CABEC had been envisioned as developing a large proposal which would encompass the research interests of several LBL and UC investigators and which would have as its theme "investigating the sequence of events from the generation and release of combustion products to their fate and ultimate effects." However, the success of such a proposal was increasingly recognized as unlikely. Further, the Center had extended activities to include research on the effects of technologies (in addition to the combustion of fossil fuels): indoor pollutants, toxic substances in surface and ground waters, and greenhouse gases in general. As a result of these and other considerations, the name of the Center was changed to the **Center for Atmospheric and Biospheric Effects of Technology (CABET)**. The revised purpose of the Center is to "investigate the atmospheric and biospheric effects of technologies, and the sources and processes leading to those effects." Within this broad mandate, the emphasis during FY88 was on developing research efforts in environmental toxicology and global climate change.

Craig Hollowell, a Senior Scientist in the Division until his untimely death in January, 1982, was the leader of our indoor air quality research program. In 1983, the Craig Hollowell Lecture Series on Energy and the Environment was established as a memorial to Craig and as a way of providing recognition to outstanding scientists in the energy and environmental fields. The first five lecturers have set a high standard. They were:

1983 **Jan A. J. Stolwijk**, Yale University
Indoor Air Pollution: Exposure and Health Effects

1984 **Tihomir Novakov**, LBL
Smoke, Soot, Fog in the Atmosphere: From London to Los Angeles and Back

1985 **Peter Schwartz**, Shell Group
What Happened to the Energy Crisis?: The

Dilemma of an Energy Decision Maker in a Dynamic World

1986 **Samuel Berman**, LBL
Shedding a Little Biophysics on Light: A New Visual Photometry

1987 **Mary O. Amdur**, MIT
Combustion-generated Acid Aerosols: An Interdisciplinary Bridge from Stack to Lung

The calendar year 1988 lecture will be given in November by Arthur Rosenfeld of LBL on *Energy Efficiency vs. Global Warming.*

Center for Building Science

The Center for Building Science provides a structure for groups in different programs but with similar interests to perform joint research, to develop new research areas, to share resources, and to produce joint publications. The Center plans future building-science research, obtains funding for research, transfers building science R&D results to industry, and serves as a point of contact for building-science work at Lawrence Berkeley Laboratory.

The Center must be viewed in the larger context of the continuing national need for research on the efficient use of energy in buildings. Buildings are the major energy consumer in the United States. In 1984, the U.S. buildings sector used $170 billion worth of energy, mainly as electricity. Of total annual U.S. electricity sales of $150 billion, most ($110 billion) was used for operating building equipment, lighting, and appliances. Use of fuels in buildings is also substantial ($60 billion of $290 billion).

Since 1973, rising energy prices and awareness have reduced our energy bills remarkably. Although since 1973 our stock of households has grown by 25% and commercial floor space has increased by 32%, primary energy use in buildings increased only 11%. Thus, energy use per square foot has fallen by 13% and $22 billion per year less is being spent than would be if historical trends in energy use had continued.

Substantial energy savings can be realized by retrofitting existing buildings and by constructing efficient new buildings. One way to estimate these potential savings is to use a "least cost" scenario that maximizes life-cycle cost effectiveness. A recent study for the state of Michigan indicates that, by the end of a 20-year period of new construction and retrofitting, a least-cost approach would save about one-third of the usual energy cost.

Building-energy research accelerates the capture of such potential energy and cost savings by 1) developing innovative concepts that lead to energy-efficient products on the market (e.g., advanced electric lighting systems, advanced windows); 2) understanding the performance of actual buildings (e.g., energy-loss mechanisms); 3) predicting the performance of new approaches (e.g., daylighting); and 4) developing the tools (e.g., computer programs) for designing efficient buildings and for understanding the effect of building standards. In addition, research is critical for understanding the human health and productivity implications of buildings (e.g., indoor air pollution and the effect of lighting on human performance). Analytic studies can help predict the impact of energy-related government policies and programs on consumers, on the building industry, and on the energy utilities.

About 140 people are involved in activities of the Center and work in four different programs: Energy Analysis, Building Energy Systems, Windows and Lighting, and Indoor Environment. The accomplishments of these programs are reported in the chapters of this annual report. Center activities for promoting energy efficiency and for obtaining research funds are described next.

California Institute for Energy Efficiency

In 1986, the Center Director and others from the Applied Science Division and the Universitywide Energy Research Group (UERG) conceptualized a research program on energy end-use and efficiency that would address the needs of California. An organizing committee was formed, and the concept was named the California Institute for Energy Efficiency (CIEE). The goals of this institute were:

1) to carry out a mid-term research program based primarily on the expertise of LBL and the UC campuses, but involving other California research and education institutions;
2) to receive financial support from California energy utilities (e.g., PG&E);
3) to receive institutional backing from the California Public Utilities Commission (CPUC) and the California Energy Commission (CEC);
4) to establish mechanisms for transferring research results to utilities; and
5) to benefit California ratepayers through lower energy costs.

At the same time the organizing committee was forming CIEE, efforts were underway to obtain funding from California utilities and commissions. Funds totalling $1.44M had been secured by the end of FY 1987; however, CIEE had not yet become an organizational entity. An organizational arrangement compatible with CIEE's intended purpose and acceptable to LBL, UERG, and the University of California Office of the President (UCOP) is being developed, and the future of CIEE as an established research institute seems assured.

Testimony

Testifying before congressional committees and before state utility commissions is an important activity of the Center for Building Science. During FY88, the Center Director gave the following testimony:

1) Before the U.S. House of Representatives Committee on Energy and Commerce, Subcommittee on Energy and Power, on conservation, competition, and national security;
2) On behalf of the State of Connecticut Office of Pol-

icy and Management, Department of Public Utility Control, regarding application of Connecticut Light & Power Company to amend its rate schedules;

3) Before the U.S. House of Representatives Committee on Merchant Marine and Fisheries, Subcommittee on Fisheries, Wildlife Conservation and the Environment, proposing energy efficiency as an alternative to draining oil from the outer continental shelf;

4) On behalf of the Conservation Law Foundation, testimony was given in the Massachusetts Department of Public Utilities investigation into the pricing of electricity which does not qualify for purchase under Massachusetts cogeneration statutes;

5) On behalf of the State of Michigan Public Service Commission regarding its hearings on the application of Midland Cogeneration Venture Ltd. for approval of capacity charges contained in a power purchase agreement;

6) On behalf of the Conservation Law Foundation of New England and the Natural Resources Council of Maine before the State of Maine Public Utilities Commission regarding the petition by the Central Maine Power Company for a certificate of public convenience and necessity for purchase of generating capacity and energy from Hydro Quebec;

7) Before the Wisconsin Public Service Commission's hearings on a new policy to improve building efficiency, reduce pollution, and avoid power plant production;

8) At the public hearing on the California Energy Commission's 1988 Conservation Report;

9) On behalf of the Conservation Law Foundation and the Vermont Natural Resources Council (Vermont Public Interest Research Group), testimony was given before the State of Vermont Public Service Board regarding least-cost investments, energy efficiency, conservation, and management of energy demand.

Details of these activities can be found in Center publications.

Least-Cost Utility Planning

During 1988, the National Association of Regulatory Utility Commissioners (NARUC) convened in San Francisco for their annual meeting. Members of the NARUC Conservation Committee were invited to Lawrence Berkeley Laboratory for a full day of presentations describing least-cost utility planning (LCUP) research conducted by Center programs; 21 NARUC members (including several commissioners) accepted the invitation. Proceedings of the meeting were later presented to all attendees. Participants reacted enthusiastically, commenting that the program was well planned and consistently engrossing.

Thanks to efforts by the Center Director and others, funding was obtained for a project to create a LCUP Information Systems Network that will update and merge technology databases from U.S. institutions such as EPRI, GRI, and LBL as well as from similar institutions in other countries. During FY88, contacts were established with representatives of EPRI, GRI, and NARUC and discussions are underway to devise a procedure for combining information in the databases of these three institutions. In addition, the establishment of a least-cost journal is being actively pursued jointly by the Center Director and the Commissioner of the Nevada Public Service Commission.

The following publications describe selected Center activities conducted between October 1987 and October 1988. A complete list of Center publications may be obtained by calling (415) 486-4834.

Huang J, Akbari H, Taha H, Rosenfeld A. The Potential of Vegetation in Reducing Summer Cooling Loads in Residential Buildings. *Journal of Climate and Applied Meteorology* 1987; 26(9):1103-1116. (LBL-21291)

Rosenfeld A. Energy-Efficient U.S. Buildings and Equipment: Progress Toward Least Lifecycle Cost. Proceedings of the Soviet-American Symposium on Energy Conservation, Moscow, June 1985. *Energy* 1987; 12(10):1017-1028.

Rosenfeld AH, Hafemeister D. Energy-Efficient Buildings. *Scientific American* 1988; 258(4):78-85.

Rosenfeld A. Testimony on behalf of the State of Connecticut Office of Policy and Management, Department of Public Utility Control, regarding application of Connecticut Light & Power Company to amend its rate schedules. December 9-10, 1987.

Mills E, Harris J, Rosenfeld A. Developing Demand-Side Energy Resources in the United States: Trends and Policies. April 1988. (LBL-24920)

Taha H, Akbari H, Rosenfeld A, Huang J. Residential Cooling Loads and the Urban Heat Island: The Effect of Albedo. *Building and Environment* 1988; 4:271-283.

Rosenfeld A. Energy Efficiency Versus Draining America. Testimony for Oversight Hearing on Oil Development in ANWR and National Energy Policy; U.S. House of Representatives Committee on Merchant Marine and Fisheries, Subcommittee on Fisheries and Wildlife Conservation and the Environment. Washington, DC, March 31, 1988.

Rosenfeld A, Mills E, Mowris R, Koomey J. Energy Efficiency, Competition, and Least-Cost Planning. Presented at the NARUC Least-Cost Utility Planning Conference, Aspen, CO, April 10-13, 1988.

Rosenfeld A. Testimony on behalf of the Conservation Law Foundation to the Massachusetts Department of Public Utilities investigation into the pricing and ratemaking treatment to be afforded new electric generating facilities which are not qualifying facilities. May 2, 1988.

Akbari H, Huang J, Martien P, Rainer L, Rosenfeld A, Taha H. Urban trees and light-colored surfaces: Inexpensive and effective strategies for reducing summer heat islands, cooling energy consumption, and global CO_2 concentration. Presented at the EPA/LBL Workshop on

Energy Efficiency and Structural Change: Implications for the Greenhouse Problem. Berkeley, CA, May 1-3, 1988.

Mills E, Mowris R. Energy Efficiency: The Progress and the Promise. Presented at the EPA/LBL Workshop on Energy Efficiency and Structural Change: Implications for the Greenhouse Problem. Berkeley, CA, May 1-3, 1988.

Rosenfeld A. Testimony on behalf of the State of Michigan Public Service Commission regarding its hearings in the matter of the Application of Midland Cogeneration Venture Ltd. Partnership for Approval of Capacity Charges Contained in a Power Purchase Agreement with Consumers Power Company, Case #U-8871. Lansing, MI, June 13, 1988.

Koomey J, Rosenfeld A. Promoting Efficiency Investments in New Buildings. Presented at the 1988 ACEEE Summer Study on Energy Efficiency in Buildings. Pacific Grove, CA, August 28-September 3, 1988. (LBL-25228)

Akbari H, Huang J, Martien P, Rainer L, Rosenfeld A, Taha H. The Impact of Summer Heat Islands on Cooling Energy Consumption and Global CO_2 Concentration. Presented at the ACEEE Summer Study on Energy Efficiency in Buildings. Pacific Grove, CA, August 28-September 3, 1988. (LBL-25179)

Harris J, Mills E, Mowris R, Rosenfeld A, Geller H, Ledbetter M. The Importance of Research and Development in Advancing Energy Efficiency. June 1988.

Rosenfeld A. Testimony on behalf of the Conservation Law Foundation of New England and the Natural Resources Council of Maine before the State of Maine Public Utilities Commission, Central Maine Power Company, regarding the Petition for Certificate of Public Convenience and Necessity for Purchase of Generating Capacity and Energy from Hydro Quebec, Docket No. 88-111. Augusta, ME, May 16, 1988.

Rosenfeld A, Mowris R, Koomey J. Energy Efficiency and Least-Cost Planning. Comments prepared for the California Energy Commission, Conservation Programs Committee, Public Hearing on the Draft 1988 Conservation Report. Sacramento, CA, July 12, 1988.

Rosenfeld A. Testimony on behalf of the Conservation Law Foundation and the Vermont Natural Resources Council, Vermont Public Interest Research Group, before the State of Vermont Public Service Board regarding the Investigation into Least-Cost Investments, Energy Efficiency, Conservation, and Management of Energy Demand, Docket No. 5270, Montpelier, VT, July 25, 1988.

Rosenfeld A, Koomey J. Promoting Efficiency Investments in New Buildings: A New Policy to Improve Building Efficiency, Reduce Pollution, and Avoid Power Plant Construction. Testimony on behalf of Wisconsin's Environmental Decade before the Wisconsin Public Service Commission's Hearings on Advance Plan 5, Docket No. 05-EP-5, Madison, WI, August 4, 1988.

Center for Atmospheric and Biospheric Effects of Technology

The Center for Atmospheric and Biospheric Effects of Technology (CABET) has continued to provide an umbrella for similarly interested groups in different programs within the Applied Science Division, other Lawrence Berkeley Laboratory divisions, and other University of California departments to 1) perform joint research; 2) develop new research areas; 3) share resources; and 4) publish together. Two major research themes that have attracted a great deal of national and international attention—environmental toxicology and global climate change—have helped to focus the activities of CABET.

Several components of CABET's global climate change activities have already been described (see Summary of Activities). In addition, at a more general level, several scientists have participated in workshops aimed at helping the Department of Energy (DOE) determine how it might best contribute to the International Geosphere/Biosphere Program (IGBP) both in the atmospheric and ecologic areas. A number of reports have been drafted, and we expect that our participation in this process will help us to play a significant role in some of these programs—particularly after they have been clearly formulated and implemented at DOE. Our interactions with the Electric Power Research Institute (EPRI) have increased significantly at various programmatic levels, mainly in response to that organization's increased interest in global climate change. We expect that, with EPRI launching a major effort in this field, we might also participate jointly in critical research and policy areas for which we have unique capabilities (e.g., with respect to cloud chambers, NO_2 generation, the role of Less-Developed Countries (LDC's) and China, ecosystem responses).

In the environmental toxicology area, we have initiated a major new effort in aquatic toxicology. Funded by both the National Institute of Environmental Health Sciences (NIEHS) and the Environmental Protection Agency (EPA), efforts are underway to identify and characterize some of the point sources of toxic effluents in the Bay Area and the molecular targets (at the DNA and reproductive levels) of toxicity in aquatic environments. Oxidative and free radical stress to cells and tissues has continued to be an important area of study for several ASD investigators who have collaborated actively with a number of other well-known groups in this field, both at LBL and throughout the San Francisco Bay Area. Recognizing the increasing necessity of placing human health risk analysis on a more fundamental scientific basis, discussions have been initiated between several investigators in the Indoor Environment Program and the Biomedical and Environmental Health Sciences (BEHS) department on the Berkeley campus; a major goal of these interactions is the establishment of a new and unique effort at Berkeley that will integrate some of the best indoor exposure models

developed at LBL with the new mechanism-based pharmacokinetic and cancer models being developed in BEHS. Most researchers today agree that without such integration, risk analysis would remain controversial at best and inaccurate at worst, with societal implications that could become enormously costly.

ENERGY CONVERSION AND STORAGE PROGRAM STAFF

Elton Cairns, Program Leader
Harvey Blanch, Deputy Program Leader
Michael Wahlig, Deputy Program Leader

Thomas Adler
Daniel Arenson
Vincent Battaglia
Paul Berdahl
Ernest Blatchley
Garth Burns
Van Carey
Douglas Clark
Thomas Colson
Daniel Crean
Linda Custer
Christian Daughton
Gregory Dow
Deborah Estis
Erik Fernandez
Richard Fish
Albert Flounders
Raymond Fong
Alan Foss
Antonio Garcia
Bruce Gilbert
Terry Grant
Edward Grens
Robert Guinn
Martin Halmann*
Donald Hanson
Otto Haas*
Gregory Hiller
Richard Hix
Raymond Ho*
Isaac Hodara*
Paul Hsuin
Arlon Hunt
Mark Isaacson
Alejandro Izquierdo
Aviezer Kertes
Hoon-Sik Kim
Hyun-Ok Kim
C. Judson King
Kim Kinoshita
Judith Klinman
Gregg Langlois
Susan Lauer
Laura Lindsay-Murphy
Kevin Lofftus
Scott Lynn
Anthony Mancuso
Frank McLarnon
Jeffrey McMillan
Fletcher Miller
Kenneth Miller
Riley Moore
Marilee Murphy
Stuart Naftel
Mindy Ng
Dan Neumann*
Jon Noring
Loree Poole
Robert Price
Michael Prince
Corie Ralston*
Saroja Ramamurthi*
Lucy Randel
John Reynolds*
Paul Ridgway
William Rixey
Dorys Rojas de Olivares*
James Rudnicki
James Russell
Richard Russo
Richard Sakaji
Robert Selleck
Hugh Salmon*
Daniel Shapiro
Susan Sharfstein
David Schurig
Jon Spear
Charlotte Standish
John Starr
Craig Stevens
Kathryn Striebel
Janet Tamada
Jerome Thomas
Albert Wang
Jeffrey Weaver
Charles Wilke
Richard Williams

*Participating Guest

ENERGY CONVERSION AND STORAGE

INTRODUCTION

The Energy Conversion and Storage Program applies chemistry and chemical engineering principles to solve problems in *a*) the production of new synthetic fuels, *b*) the development of high-performance rechargeable batteries and fuel cells, *c*) the development of advanced thermochemical processes for energy storage, *d*) the characterization of complex chemical processes, and *e*) the application of novel materials for energy conversion and transmission. Projects focus on transport-process principles, chemical kinetics, thermodynamics, separation processes, organic and physical chemistry, and advanced analysis methods.

The electrochemical energy storage and conversion project develops advanced power systems for electric vehicle and stationary energy storage applications. Topics include identification of new electrochemical couples for advanced rechargeable batteries, improvements in battery and fuel cell materials, and the establishment of engineering principles applicable to electrochemical energy storage and conversion. Major emphasis is on applied research that will lead to superior performance and lower life-cycle costs.

Research in thermochemical energy storage and conversion focuses on new and innovative approaches to the more efficient utilization of thermal and solar energy. Gas-particle suspensions are being developed for use in direct solar-thermal conversion processes, and for the catalysis of important thermochemical reactions.

Coal-related research strives to develop improved, energy-efficient methods for processing waste streams from synfuel plants and coal gasifiers. Of particular interest are new techniques to remove compounds such as H_2S, NH_3 and phenols from effluents, and the establishment of a data base for physical, chemical and biological properties of the numerous compounds that are found in such streams.

Energy-related chemistry projects seek to identify and characterize the constituents of liquid fuel system streams, and devise energy-efficient means for their separation. Also of current interest is the development of advanced methods for production of alcohols from hydrocarbon fuels; the application of novel microstructured materials to develop super-insulating windows, new ceramics, and high-temperature superconducting films; and the use of ultrasensitive optical techniques to characterize high-temperature superconductor fabrication processes and biochemical reactions.

Technology Base Research Project for Electrochemical Energy Storage*

E.J. Cairns, K. Kinoshita, and F.R. McLarnon

The Lawrence Berkeley Laboratory (LBL) is lead center for management of the Technology Base Research (TBR) Project, which is supported by the Electrochemical Branch of DOE's Office of Energy Storage and Distribution. This project's research supports DOE development of electrochemical energy conversion systems for electric vehicles and stationary energy storage. Specifically, most promising electrochemical technologies will be identified and transferred to industry and/or to another DOE program for further development and scale-up.

The TBR Project identifies new electrochemical couples for advanced batteries, determines the technical feasibility of the new couples, improves battery components and materials, establishes engineering principles applicable to electrochemical energy storage and conversion, and investigates fuel cell and metal/air systems for transportation applications. Major emphasis is given to applied research that will lead to superior performance and lower life-cycle costs.

The LBL scientists participating in the project are E.J. Cairns, K. Kinoshita, and F.R. McLarnon of the Applied Science Division; and L.C. DeJonghe, J.W. Evans, R.H. Muller, J.S. Newman, P.N. Ross, and C.W. Tobias of the Materials and Chemical Sciences Division.

Research projects conducted by subcontractors are described in the report, *Technology Base Research Project for Electrochemical Energy Storage* (LBL-25507); in-house work is summarized in the next article and in the *Materials and Chemical Sciences Division 1988 Annual Report* (LBL-26455). Highlights of the subcontracted work follow.

EXPLORATORY RESEARCH

Efforts at Argonne National Laboratory (ANL) are focused on two advanced high-temperature rechargeable battery systems: *a)* $LiAl/FeS_2$ cells containing a dense upper-plateau (U.P.) FeS_2 electrode, a Li-Al electrode, and LiCl-LiBr-KBr electrolyte (m.p. 310°C); and *b)* Na/β''-$Al_2O_3/NaAlCl_4/NiCl_2$ cells ($Na/NiCl_2$ cells). Overcharge tolerance of U.P. FeS_2 for >250 cycles in $LiAl/FeS_2$ cells at 400°C was demonstrated, and the test is continuing. The performance of $Na/NiCl_2$ cells was shown to be sensitive to electrode thickness and to Ni particle size.

University of Pennsylvania and University of Minnesota investigations into the electrochemical properties of conducting polymers showed that the hydration/dehydration of poly(ethylene oxide) [PEO] profoundly influences the ionic transport of dissolved cations such as Ni^{2+} and Co^{2+}. Hot pressing and solvent casting were successfully used to prepare thin-layer electrochemical cells containing PEO.

APPLIED SCIENCE RESEARCH

Stanford University investigated sodium alloy (Na-Sn, Na-Pb) electrodes and $NaAlEt_4$ (Et = ethyl group) liquid electrolyte as replacements for the negative electrode/β''-Al_2O_3 assembly in $Na/FeCl_2$ cells. Constant-potential plateaus were identified for various compositions of alloys at 120°C. Thin films of $FeS_{1.5}$ (1-3 μm) were produced by high-rate atmospheric-pressure chemical vapor deposition (CVD), and tests of these materials in small Li/FeS_x cells are being conducted.

Studies at the Massachusetts Institute of Technology showed that chemical stability to Li at high temperatures was improved by a "passivating" layer of Ca on the surface of glasses, which are fast-ion conductors but are susceptible to attack by Li. These glasses are being developed for use in high-performance, rechargeable Li/S cells.

The Illinois Institute of Technology (IIT) has successfully electrodeposited Mo and Mo_2C layers from a FLINAK (LiF-NaF-KF) melt. Samples of these coatings are now being evaluated by an industrial developer of Na/S cells.

Brookhaven National Laboratory (BNL) and IIT are studying the electrodeposition of Zn in electrolytes for flow batteries. BNL's EXAFS (Extended X-ray Absorption Fine Structure) studies of supersaturated zincate solutions showed no evidence of chain or polymer formation as previously reported. IIT observed that pulse-reverse-voltage charging reduces formation of dendrites and produces more coherent Zn deposits than those obtained by alternating-voltage charging.

Spectroscopic techniques are being applied at Case Western Reserve University (CWRU) and Jackson State University to characterize the surface of reactive alkali and alkaline earth metals in organic electrolytes. Electron energy-loss spectroscopy of CO_2 adsorbed on K revealed two strong bands for CO_2 vibration. Raman spectra showed bands indicative of decomposition products from reactions of Li in 2-methyl tetrahydrofuran and propylene carbonate (PC).

Johns Hopkins University observed that Fe and Ni, in highly purified PC, exhibit similar electrochemical behavior near their corrosion potentials but that differences appear at high overpotentials. Fe retains its passive behavior up to the potential (E_p) at which PC is oxidized, whereas Ni begins to pit at about 500 mV below E_p.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution, Energy Storage Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

AIR SYSTEMS RESEARCH

Research at CWRU confirmed that a transition metal oxide must be present in heat-treated organic macrocycles to obtain active catalysts for oxygen reduction. These findings were observed with the organic macrocycles: dibenzotetraazaanulene, tetramethoxyphenyl porphyrin, and octaethyl porphyrin.

Experiments at Pinnacle Research Institute demonstrated that Mg is a better substrate than glassy carbon (GC) for Zn deposition during recharge of a Zn/air cell; about 0.52 Wh/g Zn was required for Zn deposition onto a Mg substrate, whereas the corresponding value needed for a GC substrate was 0.98 Wh/g.

Work at SRI International showed that solution-phase inhibitors (*e.g.*, Bi, Ga, In, Mn, Sn) may provide an alternative to alloying for reducing the corrosion of Al in Al/air batteries. These inhibitors precipitate on the Al surface to suppress corrosion.

Los Alamos National Laboratory observed that steam-reformed methanol that was partially oxided to reduce the CO content to 10 ppm still showed significant performance losses in proton-exchange membrane (PEM) fuel cells. However, the direct injection of O_2 (2-3%) in the anode compartment of PEM fuel cells produced cell performance comparable to that obtained using CO-free fuel.

BNL's EXAFS studies of Pt electrocatalysts showed that phosphate anions are strongly adsorbed on Pt, whereas no anions are adsorbed from CF_3SO_4H electrolyte.

Advanced Electrode Research*

E.J. Cairns, F.R. McLarnon, T.C. Adler, M.J. Isaacson, K.G. Miller, S.A. Naftel, P. Ridgway, J. Rudnicki, R. Russo, and J. Weaver

The purpose of this research is to study the behavior of electrodes used in secondary batteries and fuel cells, and to investigate practical means for improving their performance and lifetimes. Systems of current interest include ambient-temperature rechargeable cells with Zn electrodes (Zn/air, Zn/NiOOH, Zn/AgO, Zn/Cl_2, Zn/Br_2, and $Zn/Na_3Fe(CN)_6$); rechargeable high-temperature cells (Li/S, $LiAl/FeS_2$, Na/S and $Na/NiCl_2$); and fuel cells. The approach used in this investigation is to study life- and performance-limiting phenomena under realistic cell operating conditions.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution, Energy Storage Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

ALKALINE ZINC ELECTRODES

Rechargeable alkaline Zn/air and Zn/NiOOH cells can be designed to deliver high specific energy and specific power, but they typically exhibit short lifetimes. The high solubility of Zn species in alkaline electrolytes tends to enhance physicochemical processes (active material redistribution, filamentary Zn growths, etc.) that degrade the cell's capacity and limit its life. Modeling and experimental investigations attempt to understand the complex transport processes within operating Zn electrodes and to characterize methods for reducing Zn species solubility in order to extend the lifetime of the Zn electrode.

A TWO-DIMENSIONAL MATHEMATICAL MODEL OF THE POROUS ZINC ELECTRODE

M.J. Isaacson, E.J. Cairns, and F.R. McLarnon

The first two-dimensional mathematical model of the porous Zn/ZnO electrode was developed, and the model predictions were compared to prior μ-electrode and cell cycling studies.[1] This model accurately predicted the influence of cell geometry and concentration gradients on the current density distribution, whereas one-dimensional models could not do so. The effect of the hysteresis in the ZnO precipitation/dissolution kinetics (*i.e.*, formation of a meta-stable supersaturated $Zn(OH)_4^{2-}$ solution during discharge) was also incorporated into the model. The ZnO precipitation rate constant could then be estimated by comparing simulation results to experimental data. The model predictions were in good agreement with experimental charge/discharge curves and μ-electrode data. The μ-electrode experiments and the model both showed that: *a*) KOH concentration changes are small during both charge and discharge, and *b*) $K_2Zn(OH)_4$ concentration gradients are larger during discharge than those during charge. The model predicted movement of Zn-active material from the middle of the electrode to the edge of the electrode, agreeing with experiments conducted in 30% KOH electrolyte in this laboratory.

The 0.42-mm-thick electrodes used in the simulation displayed a relatively uniform current density distribution, and the Zn active material was well utilized. However, concentration gradients magnify the non-uniformity of the current density distribution, and differences in the concentration field during charge and discharge cause a net movement of both ZnO and Zn metal. These differences in the concentration field result from hysteresis in the dissolution/precipitation reaction and from the presence of electrolyte reservoirs.

The results suggest that material redistribution may be minimized by the use of additives that decrease the stability of the supersaturated $Zn(OH)_4^{2-}$ solution and by redesigning the cell to minimize the effect of electrolyte reservoirs.

A MATHEMATICAL MODEL OF THE RECHARGEABLE Zn/NiOOH CELL

K.G. Miller, E.J. Cairns, and F.R. McLarnon

The one-dimensional, time-dependent model reported earlier has been implemented.[2] Designed to elucidate the cause of active material redistribution in the Zn electrode, this model takes into account transport of electrolyte species, heterogeneous reactions, kinetics, and variations in current density.

The model includes important phenomena that have been suggested as causes of Zn active material redistribution, with the exception of non-uniform current density distribution near the edges of the electrodes. To study the effects of different processes on the rate and extent of Zn redistribution, the model now simulates the Zn/NiOOH cell during the course of 20-50 deep-discharge cycles.

These simulations have yielded important conclusions. First, the dominant processes which determine the zincate $[Zn(OH)_4^{2-}]$ and hydroxide (OH^-) ion concentrations are the electrochemical reactions at both electrodes and the ZnO dissolution/precipitation reactions. Transport of electrolyte species across the membrane is generally much more important than transport in the direction parallel to the plane of each electrode. Also, transport of species in the pores of the electrodes is primarily due to convection, with diffusion and migration contributing little. Second, the electrolyte becomes supersaturated with $Zn(OH)_4^{2-}$ at the end of the first cycle, and the $Zn(OH)_4^{2-}$ concentration remains at elevated levels during subsequent cycles (compared to levels during the first cycle). Third, at the end of the first cycle, precipitation of ZnO in the NiOOH electrode has already occurred. After ZnO precipitation is initiated in the NiOOH electrode, this ZnO never redissolves completely, and the amount of precipitated ZnO increases as the cell is cycled. Finally, from preliminary studies, the most sensitive parameters in determining the Zn redistribution pattern are the values of the rate constants in the ZnO precipitation/dissolution reactions.

IN SITU SPECTROSCOPIC CHARACTERIZATION OF ZINC ELECTRODE PROCESSES

J. Weaver, E.J. Cairns, and F.R. McLarnon

The rates of solid-phase precipitation and dissolution in porous Zn electrodes are known to play important roles in the life-limiting material redistribution processes in this system. Neither the rates of precipitation/dissolution nor the identity of the precipitating/dissolving species are known. We are applying photothermal deflection spectroscopy (PDS) as a powerful, *in situ* technique to characterize this electrode. A model pore electrode system, amenable to microscopic and spectroscopic study, is being employed to simulate a real pore that exists in a rechargeable Zn battery electrode.

Two features of the model pore electrode are under investigation: *a*) the species formed on the electrode surface, and *b*) the concentration gradients generated in the electrolyte adjacent to the electrode. During FY 1988, PDS was used to study concentration gradients in a model pore electrode, and conventional light microscopy was used to observe surface species that form on the electrodes.

The electrodes in the model pore system are mounted in clear polished acrylic, which is in turn supported in a quartz optical cuvette. Alkaline electrolyte, saturated with ZnO, is kept in an electrolyte compartment. The size of the electrolyte compartment can be adjusted to a range of model pore dimensions by inserting spacers of various thicknesses between the acrylic support and the quartz cuvette. The entire cuvette arrangement is mounted on a support which allows alignment to submicron precision.

Several constant-current experiments were carried out, during which PDS data were collected at various locations along the length of the electrode. As expected for anodic Zn oxidation, PDS experiments indicated that the concentration of soluble Zn species is higher near the electrode surface, and for cathodic Zn electrodeposition the reverse is true. For both anodic and cathodic experiments, the gradients became smaller near the closed end of the model pore electrodes (*i.e.*, away from the counter electrode). These results are now being compared with those predicted by a one-dimensional numerical model of the transient diffusion processes in this system.

The progress of reactions on the electrode surface has also been observed with a light microscope. A grey oxide film typically grows toward the closed end of the model pore anode during the course of the experiment, in agreement with earlier observations by others.

METHODS TO IMPROVE THE LIFETIME OF THE ZINC/NICKEL OXIDE CELL

T.C. Adler, F.R. McLarnon, and E.J. Cairns

Zinc redistribution is a major failure mode of the Zn/KOH/NiOOH cell and is associated with the high solubility of the zincate species in the alkaline electrolyte. A typical procedure for preparing a Zn/NiOOH cell to undergo repeated charge/discharge cycling is to subject it to extended low-current-density charges and discharges ("formation cycles") that establish a Zn metal reserve and "condition" the NiOOH electrode. A series of formation-cycle experiments has shown that as much as 15% of the original Zn is deposited in the NiOOH electrode during the first few formation cycles; this surprising result indicates that Zn redistribution is well established before normal cell cycling even begins!

Three approaches have successfully reduced Zn redistribution: *a*) reducing the concentration of zincate species in the electrolyte by reducing its alkalinity, *b*) binding the Zn-active material in a nearly insoluble calcium zincate complex, and *c*) employing optimized cell charging waveforms. Efforts during FY 1988 have been directed toward combining these three approaches.

Electrode/electrolyte combinations that exhibit low Zn species solubilities often exhibit high Zn electrode overpotentials when the cell is charged, and concomitant zincate-ion gradients in the electrolyte increase the likelihood of dendritic shorting. By maintaining the cell voltage at 1.93 V and reducing the cell current accordingly, the problems associated with high-overpotential charging can be avoided. The LBL computer-controlled electrochemical cell test-cycling system was adapted to provide this constant-voltage, limited-current mode of charging (CVLC); subsequently all cells have been charged in this mode.

Prior attempts to combine alkaline-fluoride electrolytes (which exhibit reduced zincate-ion solubility and are compatible with pure Zn/ZnO electrodes) with Zn-Ca electrodes showed inconsistent results, apparently due to difficulty in forming the calcium-zincate complex in this electrolyte. During FY 1988, several Zn-Ca/KOH-KX/NiOOH cells (X=halide) were constructed and tested. These cells exhibited problems during formation cycles, probably because of reduced availability of soluble zincate ion for reduction during charge. This problem was alleviated by first forming the Zn-Ca electrode in a cell containing an electrolyte with a high Li-ion content (KOH-KX electrolytes exhibit reduced Li ion solubility). Low-zincate-solubility electrolyte was then added to the cell, and the cell was cycled successfully in CVLC mode. Starved-electrolyte cells prepared in this manner are now being tested.

HIGH-TEMPERATURE CELLS

The high-temperature Na/S cell offers very good performance, and recent improvements to the process for manufacturing the ceramic β''-Al_2O_3 electrolytes indicate that acceptable cell lifetimes may be realized. However, the performance of the sulfur electrode has not been optimized, and the phenomena which govern its operation are poorly understood. In addition, Na/S cells cannot tolerate overcharge and overdischarge, a problem that complicates the design of cell-string configurations for battery applications. Ongoing work is aimed at developing and confirming an advanced mathematical model of the sulfur electrode and exploring variants of Na/S (and Li/S) cells that can tolerate limited overcharge and overdischarge.

MATHEMATICAL MODELING OF THE SODIUM/SULFUR CELL

S.A. Naftel, F.R. McLarnon, and E.J. Cairns

A comprehensive model of the sulfur electrode in Na/S cells has been developed.[3] The cell being modeled is of the tubular central-sodium type, and it incorporates a thin layer of α-alumina felt around the β''-alumina solid electrolyte in order to prevent deposition of sulfur on the solid electrolyte during cell charge. The model, consisting of a set of non-linear PDE's, describes the diffusion, migration, and convection processes that take place during operation of such a cell. The linearized equations are solved on a digital computer *via* implementation of the Newman-IAD method, a finite-difference technique for solving second-order linear PDE's.

The model was written in FORTRAN 77 and is being debugged; significant results are expected during FY 1989. An attempt will be made to predict the effect of various charge-discharge regimens upon cell operation.

FUEL CELLS

Fuel cells can be designed to exhibit acceptable lifetimes for a number of applications, and a handbook describing the status of fuel cells is available.[4] However, the performance of the O_2 electrode in fuel cells requires improvement, and development of an efficient direct-methanol fuel cell would represent a major advance over reformed-hydrocarbon fuel cells.

APPLICATION OF PHOTOTHERMAL DEFLECTION SPECTROSCOPY TO CHARACTERIZE DIRECT METHANOL ELECTROOXIDATION

J.D. Rudnicki, R.E. Russo, O. Haas, F.R. McLarnon, and E.J. Cairns*

Photothermal Deflection Spectroscopy is being used to study electrochemical interfaces.[5] PDS is a versatile, *in situ* technique which measures both absorption of light at the electrode surface and electrolyte concentration gradients formed near the electrode surface. By measuring the absorption of light at the surface as a function of wavelength, the absorption spectrum of the surface is determined. Such a spectrum can be used to identify the species on the electrode surface. The sensitivity of the technique is high enough to detect the absorption of light and concentration gradients due to the formation of less than one molecular layer of species on an electrode surface. The information provided by PDS helps determine reaction mechanisms, and with this knowledge methods to improve the efficiencies of electrode reactions can be formulated.

Platinum electrodes have been studied because of their high electrocatalytic activity for methanol oxidation, and supported-Pt electrodes would be good candidates for use in direct-methanol fuel cells. The Pt surface can be modified by the presence of a small amount of another species on the electrode surface (either adatoms or admolecules) resulting in a synergistic increase in the catalytic activity. One method of accomplishing this modification is underpotential deposition (UPD), and the UPD of Pb on Pt has been studied. The PDS results provided information which showed that the UPD process is different than that which would be expected from standard

* Paul Scherrer Institute, Switzerland

electrochemical experiments. The study of UPD of other species on Pt is in progress.

The versatility of PDS has been expanded. Many types of electrodes, including smooth Pt, Cu, polymer films on carbon or a fine screen, and porous UO_2 have been studied as electrode surfaces. Improvements in the signal-to-noise ratio have been made, and increased sensitivity has allowed the experimental data to be obtained in a shorter time. Work has also been started to expand the spectral range of PDS into the near- and mid-infrared.

REFERENCES

1. Isaacson MJ, McLarnon FR, Cairns EJ. Mathematical model of the secondary current distribution mechanism for Zn material redistribution. Paper No. 7 presented at the *174th Meeting of the Electrochemical Society*, Chicago, IL, 1988.
2. Miller KF, McLarnon FR, Cairns EJ. Mathematical model of the secondary Zn/NiOOH cell. Paper No. 6 presented at the *174th Meeting of the Electrochemical Society*, Chicago, IL, 1988.
3. Naftel SA, McLarnon FR, Cairns EJ. Studies of the sulfur electrode in sodium/sulfur cells. Paper No. 81 presented at the *170th Meeting of the Electrochemical Society*, San Diego, CA, 1986.
4. Kinoshita K, McLarnon FR, Cairns EJ. *Fuel cells–a handbook.* Report No. DOE/METC-88/6096, 1988. (PUB-644)
5. Russo RE, Rudnicki J, McLarnon FR, Cairns EJ. Versatile optical probe beam deflection spectrometer for *in-situ* spectroelectrochemistry. Paper No. 111 presented at the *39th Meeting of the International Society of Electrochemistry*, Glasgow, Scotland, 1988.

Direct Solar Thermal Conversion Processes*

A. Hunt, I. Hodara, F. Miller and J. Noring

This research explores advanced concepts in the direct conversion of concentrated solar energy to thermal and chemical forms. Of the four research areas, two involve purely solar thermal processes; the others address the solar heating of catalysts to drive useful chemical reactions. The unifying theme is the absorption of concentrated solar energy by small particles and its conversion to other forms. The concept of entrained particle absorbers was first demonstrated in 1982 with the solar test of the Small Particle Heat Exchange Receiver (SPHER). This approach may be used to heat gases to high temperatures for driving turbogenerators and for supplying heat for industrial processes; it may also be used to convert solar energy to chemical forms suitable for storage or transport.[1]

RADIANT HEATING OF GAS-PARTICLE SUSPENSIONS

This research was undertaken to understand the thermal and optical processes in the radiant heating of gas-particle mixtures. In FY 1988, we completed development of a cylindrical receiver model and related experimental work to study the operation of an idealized receiver system. Our goal was to understand the absorption of radiation by the particles, the heating and expansion of the gas, and the resulting temperature, density, and flux profiles within a solar receiver. The results of our research will provide a basis for designing future direct-absorption receivers.

An analytic model of a long cylindrical receiver was developed to predict temperature and flux distribution in a gas-particle suspension flowing along the axis of the receiver. The model provides information regarding gas densities and the effects of flow direction and gives detailed performance predictions for our experimental receiver, which was constructed to test the model.

The receiver system consists of a vacuum-insulated cylindrical receiver, carbon-particle generator, light source, and associated instrumentation. The light source produces a collimated beam of light along the axis of the tube with a peak intensity of over 80 suns. Carbon particles are mixed with air and directed in either a co- or counter-current flow direction with respect to the direction of the incident light. Thermocouples measure the temperature profile along the entire axis at 6 different radial positions and at fixed points within the receiver. The receiver was completed in FY 1988 and the measurements were compared with the model predictions.

There was general agreement between the modeled and experimental results for the counter-current case but the experiment showed more rapid heating than predicted for the co-current case. Much of the difference can be attributed to non-idealities in the experiment, but further research is required to resolve the remaining discrepancies.

CARBON-PARTICLE ABSORBERS IN LIQUID SALTS

The DOE Solar Thermal Program is developing an advanced direct-absorption receiver based on a liquid medium of Na/K nitrate salt for heat transfer and storage. The salt flows over a plate exposed to concentrated solar radiation from a field of heliostats. Because the pure salt is transparent to solar radiation, current designs call for the salt to be doped with cobalt oxide particles. We investigated the use of carbon particles as an alternative absorber. They are less abrasive and are slowly oxidized in the hot salt. Oxidation of the particles effectively eliminates problems of agglomeration and settling encountered with the cobalt oxide particles. A hot stage transmissometer was designed and built to study the oxidation, agglomeration, and settling properties of the carbon particles.

Calculations compared the mass loading of carbon and cobalt oxide as a function of particle size. On the basis of weight, our calculations showed carbon to be a better absorber than cobalt oxide.

RADIANTLY HEATED CATALYSTS FOR THERMOCHEMICAL ENERGY STORAGE

This research explores the use of concentrated sunlight to initiate endothermic catalytic reactions in gases for high-temperature thermochemical energy storage cycles. Direct radiant heating of catalyst particles to drive gas reactions has several important advantages. Enhanced heat transfer occurs because heat is supplied directly to the reaction site (in contrast to conventional reactors, where heat is supplied through pipe walls and thereby leaves the catalyst the coolest part of the system). A radiantly heated catalyst particle becomes the hottest part of the reactor, dramatically increasing the reaction rate. Additionally, a semiconducting catalyst particle can photocatalyze the reaction because the absorbed photons produce energetic photocharges. In small particles, these charges can reach the gases adsorbed on the surface to initiate the reaction.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Systems Research, Energy Storage Division through the Solar Energy Research Institute, Sandia National Laboratories, and Battelle Pacific Northwest Laboratory, through the U.S. Department of Energy under Contract DE-AC03-76SF00098.

We studied the endothermic dissociation of SO_3 to SO_2 and O_2 as a means of thermochemically storing solar energy. Experiments used hematite (iron oxide) particles fixed on a substrate and illuminated with a solar simulator. We constructed a new system for SO_3 storage and transfer and fabricated a new reaction cell. Experiments confirmed that the rate of reaction was enhanced by radiant heating as compared to isothermal heating in a furnace.

RADIANTLY HEATED CATALYSTS FOR ENERGY TRANSPORT

We investigated the feasibility of direct radiant reactors for the chemical transport of energy. In this concept, individual solar concentrators convert solar energy to chemical energy. The energy-rich gases from the collectors are piped at ambient temperatures and are combined at a central conversion site where they pass over a catalyst to produce high temperatures to drive a steam-Rankine cycle.

The reaction studied was the CO_2 reforming of methane over a catalyst at high temperature to produce H_2 and CO. Analytic models of the optical, thermal, and chemical interactions were formulated. Reticulated alumina, alumina aerogel, and fiber arrays were considered as substrates for the absorbing rhodium catalyst particles. We analyzed the mass transport, optical, and thermal properties of the reactor designs.

The uncatalyzed CO_2 reforming of methane was studied experimentally. The results of these experiments showed that the reaction may be carried out without a catalyst if sufficiently high temperatures are achieved.

In FY 1989, our solar thermal research will continue by carrying out collaborative projects with the German aerospace organization (DFVLR). The first project will quantify the losses from a radiantly heated gas-particle receiver. The second project will measure the effects of concentrated solar radiation on carbon particle oxidation rates.

REFERENCES

1. Hunt AJ, Hodara I, Miller FJ, and Noring, JE. Direct absorption receivers for catalyzing chemical reactions. *Proceedings of the 4th International Symposium on Research, Development and Applications of Solar Thermal Technology,* Santa Fe, NM, 1988.

Microstructured Materials*

A. Hunt, F. Hibbler, and K. Lofftus

This research develops new microstructured materials *via* advanced chemical processing. Liquid organo-metallic compounds are reacted to form a solid network that contains solvent. The solvent is then removed without changing the microstructure by a supercritical drying technique developed at LBL. A low-density, porous solid called "aerogel" results. Several single- and mixed-metal oxide compositions were made this way using different starting compounds. Three projects employ this technique: one develops silica aerogel for insulating windows; another explores the preparation of new ceramic materials for high temperature applications; and a third, new project, is exploring the preparation of high critical point superconductoring films using sol-gel processing.

SILICA AEROGEL, A TRANSPARENT SUPERINSULATOR

Silica aerogel is a transparent, porous insulating solid with many applications. We have developed aerogel as a transparent insulator for high-thermal-performance windows (R-20 per inch). Three major technological barriers to its commercialization have been overcome in the past six years of research and development at LBL. A safer, more economical supercritical drying process was developed and patented, the clarity of aerogel was improved, and methods to produce good-quality aerogel with alternate non-toxic starting compounds were developed.[1] In addition, economic studies indicated that mass-produced aerogel will be a cost effective insulator. This year's activities involved primarily scale-up and technology-transfer.

A new large autoclave for CO_2 substitution and supercritical drying of samples up to 12 inches square was constructed and tested. Instrumentation was developed to monitor the fluid level and composition in the autoclave. New molding techniques were developed and large alcogel samples were prepared for drying. The dried aerogel samples were encapsulated between glass, and several were evacuated.

The last stage of this project included technology transfer to private industry. Encouraged by the DOE tech-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Solar Heat Technologies, Solar Buildings Division, and the Office of Energy Systems Research, Energy Conversion and Utilization Technologies (ECUT) Division, and the Office of Energy Storage and Distribution of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

nology transfer program, Quantum Optics, Inc. was founded to commercialize the manufacture of aerogel products in the United States and Canada using the CO_2 substitution process. A key first application of aerogel may be for refrigerator insulation.

POROUS MICROMATERIALS DEVELOPMENT

Micromaterials research at LBL develops new methods to produce microporous materials and precursors based on sol-gel chemistry and supercritical solvent extraction techniques. These techniques have enabled us to create new and unusual materials. Low-density materials with controlled microporosity promise applications including high-temperature insulators, porous materials for filters, catalyst substrates and superconducting aerogels. New composite ceramics may be possible because very fine-grained aerogels have significantly lower sintering temperatures[2] than conventional ceramic powders, thereby reducing the tendency for the components to react with each other.

During FY 1988, we improved methods to prepare mixed-oxide ceramic materials, studied the effects of varying solvents and pH on microstructure, and developed analytic techniques to study the structural development of gel materials.[2] Research into the production of bulk superconducting YBCO aerogels was also carried out. New methods to prepare zirconia alcogels were developed and zirconia aerogels were prepared using the supercritical drying process.

SOL-GEL PROCESSING FOR SUPERCONDUCTING CERAMIC FILMS

A new project in the chemical fabrication of superconducting materials using sol-gel processing was initiated this year as part of the high-T_c thin film research effort at LBL. This approach offers the advantages of inexpensive fabrication methods for coating tapes and fibers, lower processing temperatures, very fine structure, and good homogeneity. The project, which started late in FY 1988, began exploring two approaches to preparing starting materials for YBCO films. In one approach separate alkoxides of yttrium, barium, and copper are prepared and mixed, before controlled hydrolysis is carried out. Alternatively, mixed alkoxides of two or three of the metals are prepared before hydrolysis. Transesterification methods were developed to prepare liquid copper alkoxide starting compounds.

The porous micromaterials area will concentrate on preparing composite aerogel materials and improved zirconia aerogels. The superconducting film project will explore the preparation of YBCO and other high-T_c compounds.

REFERENCES

1. Hunt AJ, Lofftus K. "Silica aerogel, a transparent high performance insulator," *Proceedings of the Intern. Solar Energy Society World Congress*, Hamburg, Germany, 1987.
2. Rahamam MN, DeJonghe LC, Shinde S, Tewari PH. "Sintering and microstructure of mullite aerogels," submitted to *J. Am. Ceramic Soc.* 1987; LBL-23529.
3. Hunt AJ, Lofftus K. "Process considerations in monolithic aerogels," *Mat. Res. Symp. Proceedings* 1988; 121:679-684.

Light Scattering Studies*

To study how light interacts with microstructures, we are conducting basic experimental and analytical studies of light scattering. In addition to the scattering measurements carried out in conjunction with our solar thermal conversion and microstructured materials research, we also have several projects to investigate light scattering in the biological sciences.

OPTICAL MEASUREMENTS OF THE INTRACELLULAR POLYMERIZATION OF HbS

A. Quintanilha, A. Hunt, K. Lofftus, H. Salamon, and R. Macy

Using a new, real-time light-scattering technique, we are measuring the kinetics of intracellular polymerization of Hemoglobin S (HbS) in red blood cells of individuals affected by sickle cell disease. This polymerization appears to be a major factor in capillary occlusion and crisis in the disease. In the kidney (frequently damaged in sickle cell disease) intracellular HbS polymerization is stimulated by dehydration, deoxygenation, and increased acidification; we have therefore simulated these conditions *in vitro* to study their effects on HbS polymerization in very dilute suspensions of red blood cells. The polarization-sensitive light-scattering technique developed earlier was used to measure the degree of polymerization.[1]

Our results indicate that the amount of induced circular polarized light, measured as a function of angle, increases when cells are placed in the dehydrating hypertonic medium representing the kidney environment. Furthermore, successive cycles of deoxygenation-reoxygenation appear to induce progressively larger steady-state values of this component of the scattered light. Comparison of our results with published data[2] on the amount of polymerized HbS measured using nuclear magnetic resonance (NMR) spectroscopy have been encouraging. A recently developed theoretical basis for our observations[3] shows that our results can be predicted using scattering theory.

Two additional observations are important in the pathophysiology of patients affected by sickle cell disease or sickle cell trait: *a)* our finding that the rates of polymerization and depolymerization as a function of changing

*This work was supported by the National Institutes of Health through the National Heart, Lung and Blood Institute, and the Environmental Sciences Programs Directorate of the Office of Naval Research, through the U.S. Department of Energy under Contract DE-AC03-76SF00098.

oxygen tension are different; *i.e.*, the rate of polymerization is much slower than the rate of depolymerization; and *b)* red cells from subjects with sickle trait, despite their significantly lower levels of HbS, show evidence of polymerization at low oxygen tensions and in hypertonic media. The first observation is important in determining whether the transit time of red cells through the kidney (~24 sec) is enough for polymerization of HbS to occur; the second observation can probably be related to kidney function abnormalities that develop in sickle trait patients.

MODELING BIOLOGICAL PARTICLES TO PREDICT OPTICAL PROPERTIES OF THE OCEAN

A. Hunt, M. Quinby-Hunt, K. Lofftus, and D. Shapiro

This project combines a modeling and experimental approach to study light scattering in the ocean. Measurement of the intensity and polarization of scattered light as a function of angle can be used to investigate the nature of the particles and to predict the propagation of light in the ocean. The particle population in the ocean is often dominated by live organisms of defined size, shape, and optical properties. Using various theories, we can predict light scattering from such organisms.

Approximate and exact models were implemented as computer programs to predict light scattering variously shaped particles. Using Mie theory, rigorous calculations of scattering from spherically symmetric particles were performed for unrestricted particle size and optical properties. Models based on Rayleigh-Debye theory were used for a restricted range of sizes and optical properties to predict scattering for spherical and nonspherical shapes. The range of validity of the non-rigorous theories was determined by comparing the results with rigorous theories for spherical geometries.[4]

The scattering properties of single, immobilized marine organisms were measured.[5] Cells of the dinoflagellate *Prorocentrum micans* were immobilized and measured in a transparent silica gel. The technique provides a convenient method to perform scattering or other optical measurements on immobilized cells without interference of a substrate in a liquid medium.

In FY 1989, the kinetics of HbS polymerization will be studied in red cells containing differing amounts of HbS, HbF, HbA. We plan to investigate whether a history of oxidative stress to these red cells (with and without polymerized HbS) affects their rheological properties. We will also use other components of the scattered light to distinguish between intracellular polymerization of HbS and the resulting shape changes of the cells.

Models will be used to predict the complete scattering behavior of well characterized marine organisms. Populations of several marine organisms will be cultured, measured, and compared to the model predictions to determine the sensitivity of the technique to characterize marine populations in the ocean.

REFERENCES

1. Hunt AJ, Lofftus KL, Quintanilha A. Optical measurements of the intracellular polymerization of HbS. *Blood* 1987; 70:62a.
2. Noguchi CT, Torchia DA, Schechter AN. *Proceedings of Natl Acad Sci*, 1980; 77:5487.
3. Tinoco I, Nickols W, Maestre MF, Bustamante C. *Ann. Rev. Biophys. Biophys. Chem*, 1987; 16:319.
4. Quinby-Hunt MS, Hunt AJ. Effects of structure on scattering from marine organisms: Rayleigh-Debye and Mie predictions. *Proceedings of Ocean Optics IX*, 4-8 April 1988, Orlando, FL.
5. Lofftus KD, Hunt AJ, Quinby-Hunt MS, Livolant F, Maestre M. Immobilization of unicellular marine organisms for optical characterization: a new method, *Proceedings of Ocean Optics IX*, 4-8 April 1988, Orlando, FL.

High-Temperature Superconducting Films: Electrical Characterization*

P. Berdahl and L. Williams

This new research on high-critical-temperature superconducting films, initiated in May, 1988, focuses on a.c. electrical characterization of the films. The required measurements include resistance *vs* temperature and critical current *vs* temperature. The critical current is generally defined as the maximum current that the superconductor can carry before a measurable resistance appears. The magnetic field dependence of the critical current density will also be obtained. Measurements of a.c. and d.c. magnetic susceptibility will be performed.

After some analysis and literature review, an automated a.c. electrical characterization technique was chosen which uses low-frequency excitation and phase-locked synchronous amplification to measure the small voltages required. A suitable closed-cycle helium refrigerator and cryostat were ordered to support the measurements. The synchronous detection scheme permits smaller voltages to be measured than is the case with d.c. techniques. Furthermore, the range of frequencies and magnetic fields employed (*e.g.*, 5-1000 Hz, 10^{-2} to 10 tesla) are those expected for applications of superconductors in future electric power systems.

The basic electrical characterization measurements described here primarily support the investigators syn-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution, Energy Storage Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

thesizing high-T_c films. However, in FY 1989, we will begin to investigate details of the onset of resistance in the presence of magnetic fields, a phenomenon poorly understood due to the motion of magnetic flux lines. To obtain evidence for weak current links in the films, we will also examine the relation between critical currents measured by transport techniques and those measured by magnetization techniques.

High-Temperature Superconductors: Fundamentals and Their Applications*

P. Berdahl

This work was a part of an extensive multilaboratory technology assessment entitled "Assessment of Energy Productivity Applications of High-Temperature Superconductivity." The purpose of the work was to provide an overview of selected applications of superconductivity, with emphasis on fundamental processes and novel concepts. The balance of the larger Assessment included analyses of various technological areas: motors, transportation, materials production, separations technology, electromagnetic pumping, magnetic heat pumping, materials fabrication, and power electronics. Thus, the work reported here provided an overview of the technologies, with emphasis on basic physical principles and how these principles constrain technology development. Further, the analysis was extended to include study of the emerging material properties of new superconductors.

Magnetic pressure provides an important illustrative example of how physical principles constrain technology development. Most electrical applications of superconductivity utilize electromagnets. The design of any electromagnet requires that provision be made for structural support to contain the magnetic field. For an ordinary iron-core electromagnet with copper windings, with a field of 1 tesla, this pressure is only 400 kPa (60 psi). However, this pressure is proportional to the square of the field, so that for a high-field superconducting solenoid, containment of the magnetic pressure is a major problem. At 20 tesla, the record for a (very low temperature) superconducting solenoid, the pressure is larger than that at the bottom of the ocean.

A result of the analysis of materials properties is illustrated (Figure). Most applications require current densities of 10^5 A cm^{-2} or above, at fields above 1 tesla. Therefore, except possibly for thin films, additional materials research is required to raise current-carrying capacity of

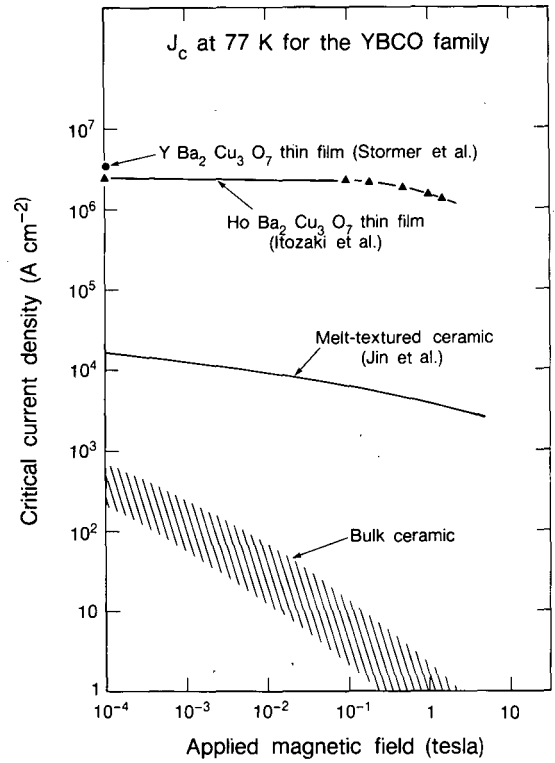


Figure. Critical current measurements *vs* applied magnetic field for a high-temperature superconducting material at 77 K (XBL 8811-9783).

YBCO (*i.e.*, $YBa_2Cu_3O_7$) before this material can be used in applications. The present situation with respect to other high-temperature superconductors is similar.

Solid State Radiative Heat Pump*

P. Berdahl

Work on this novel concept for cooling was largely concluded in FY 1987. However, publication and presentation of the results extended into FY 1988.

The Solid State Radiative Heat Pump concept utilizes non-equilibrium infrared radiation flows to produce radiative cooling and heating effects. The non-equilibrium radiation flows are caused by non-equilibrium populations of electrons and holes, produced electrically in narrow-bandgap semiconductors. The quantum efficiency for non-equilibrium electron-hole pairs to produce photons is

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Systems Research, Energy Conversion and Utilization Technologies (ECUT) Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution, Energy Storage Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

a key material figure of merit for prospective heat pump materials. A comprehensive study of quantum efficiency for radiative recombination in InSb was published.[1] Efficiencies as high as 5% were achieved at room temperature by the use of p-type (Cd) doping.

From a slightly different perspective, production of a radiative cooling effect by reducing the ordinary thermal emission from a semiconductor can be regarded as "negative luminescence": when electrically excited, system emits less infrared radiation than it does when unexcited.[2,3]

REFERENCES

1. Berdahl P. Galvanomagnetic luminescence and the quantum efficiency of radiative recombination of InSb. *J. Appl. Phys.* 1988; 63:5846-5858.
2. Berdahl P, Malyutenko V, Morimoto T. State of the art of negative luminescence, in *Proceedings of the Fourth Int. Conf. on Infrared Physics.* 17-23 (Zurich, August, 1988).
3. Berdahl P, Malyutenko V, Morimoto T. Negative luminescence in semiconductors. *Infrared Physics* (in press).

Processing of Condensate Waters from Coal Gasification*

C.J. King, T. Grant, and L. Poole

Condensate waters from low-temperature coal-gasification processes contain large amounts of dissolved phenols, ammonia, and acid gases. The goal of this project has been to develop effective and economical physicochemical treatment technology for removing these substances.

IRREVERSIBLE ADSORPTION OF PHENOLS ONTO CARBON

Adsorption of phenols by carbon is hampered by incomplete regeneration and consequent needs for adding fresh carbon. We have shown that irreversible adsorption of phenols is the result of oxidative coupling reactions accelerated by the carbon surface. Methods used included mass-spectrographic identification of reaction products and determination of the effects of temperature, pH, type of phenol, type of carbon, and various chemical treatments of the carbon surface. Irreversible adsorption can be reduced by use of low temperature, low pH, frequent generation, mild oxidation of the carbon, and an oxygen-free environment.

EXTRACTION OF AMMONIA WITH LIQUID ION EXCHANGERS

Cyanex 272, a commercial phosphinic acid extractant (American Cyanamid Corp.), has been shown to have optimal acidity for extraction of ammonia from the highly buffered condensate waters. Stripping and thermal degradation studies have established the appropriate range of temperatures for regeneration by stripping of ammonia from the extract.

*This work was supported by Program Development Funds through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Removal of H_2S from Coal-Derived Gases*

S. Lynn, T. Colson, R. Hix, and C. Stevens

When coal is gasified, most of its sulfur is converted to H_2S and must be removed before the gas can be used as a fuel or as synthesis gas. The UCB Sulfur Recovery Process (UCBSRP) is being developed as a general method for removing H_2S from gases. The H_2S is absorbed in a polyglycol ether, then reacted in the liquid phase with SO_2 to form marketable elemental sulfur and water. The process allows high specificity and flexibility; H_2S can be reduced to the part-per-million level or below in the presence of CO_2 and the other components of gasified coal. The CO_2 may be left in the original gas stream or it may be co-absorbed and recovered as a separate, sulfur-free product. The process thus has application both to syngas and hydrogen production from O_2-blown gasifiers and to power production using an air-blown gasifier.

PROCESS CONFIGURATION STUDIES

Two major goals of this project are to demonstrate the feasibility of replacing conventional industrial gas treatment technology with the UCBSRP technology and to compare the costs of the UCBSRP with those of conventional processes. One promising application of the UCBSRP is the removal of H_2S and CO_2 from a synthesis gas after a water gas shift (WGS) reactor in a process for producing high purity hydrogen.

In the production of high-purity hydrogen from gasified coal (Figure), the effluent from coal gasification is quenched with water to remove NH_3, HCl, and particulates and to cool the gas to about 430°F. To increase the H_2 content of the gas, the gas is fed to a WGS reactor, where CO is reacted with H_2O to form CO_2 and H_2. In addition, this reactor also converts some of the COS in the

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization, Division of Surface Coal Gasification of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

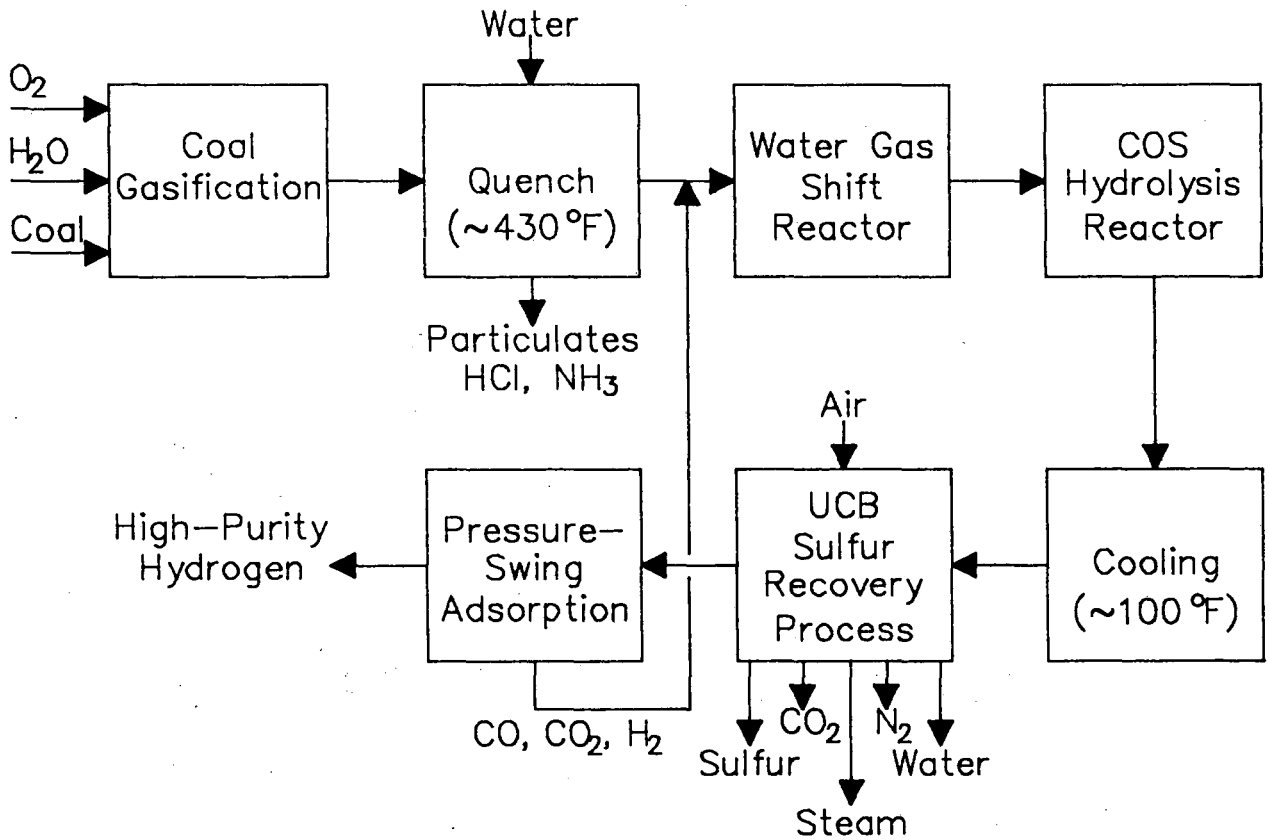


FIGURE. Block flow diagram proposed for producing high-purity hydrogen from gasified coal (XBS 8811-3939).

gas to H_2S via hydrolysis. The gas is then fed to a COS hydrolysis reactor to complete the conversion. This gas is cooled to about 100°F and sent to the UCBSRP where the H_2S and CO_2 are recovered as elemental sulfur and a purified (99+%) CO_2 stream. The treated gas from the UCBSRP is then fed to an adsorption unit for final purification. The products from the adsorber are a high-purity (99.999+%) H_2 stream and an impurity stream containing inert gases (N_2 and Ar) and any unreacted CO. Part of this stream may be recycled to the WGS reactor to recover CO, but the remainder must be purged to remove inert gases from the system.

SULFUR CRYSTALLIZATION

A major potential advantage of the UCBSRP is the purity of the crystalline sulfur that is produced. The sulfur crystallizes from solution both as a result of cooling and as a result of chemical reaction between H_2S and SO_2. In the former case, the degree of supersaturation is relatively low because the solubility of sulfur in the solvent varies only a few grams per liter over the temperature range of interest. A substantially higher concentration of sulfur can result from the chemical reaction.

The crystallizer consists of a well-stirred 2-liter vessel. Hot saturated feed enters at the top, and the vessel walls are cooled. Cold effluent exits at the bottom of the vessel as a sulfur/solvent slurry. A sample of the effluent slurry is collected when the system is at steady state and the size distribution of the sulfur crystals is determined. The first set of experiments, in which only the residence time was varied, indicated that the mixed-suspension, classified-product-removal (MSCPR) model can be used to correlate the data. Changes in residence time produce changes in nucleation and growth through their common driving force: super-saturation. The effect of supersaturation manifests itself in the general slope of the curves when the data are plotted. Although the slurry density changes slightly with residence time for a MSCPR crystallizer, large changes in slurry density were made by altering the feed temperature in the second set of experiments.

The addition of water to the solvent is equivalent to reducing the water-free solvent temperature with respect to sulfur solubility. Increasing the water concentration in the solvent should therefore produce a variable slurry density effect similar to that when the crystallizer feed temperature is reduced. Although the growth rate remains relatively invariant for different water concentrations with similar residence times, the nucleation rate increases less with increasing growth rate (decreasing residence time) when water is present.

ABSORPTION WITH CHEMICAL REACTION

Tray efficiency data are needed for two process situations. In one, H_2S at very low concentration is being absorbed by a chemically reactive solution of SO_2. In the other, gaseous SO_2 in the low parts-per-million concentration range is absorbed by lean process solvent. Both are of interest for using the UCBSRP to effect stringent sulfur removal. The equipment consists of a single sieve tray (or section of packed column) placed in a test section through which gas and liquid streams pass. Murphree tray efficiencies are determined from the mass balances and previously obtained solubility data. During FY 1988, this equipment was used to determine tray efficiencies for SO_2 absorption while varying liquid flow, gas flow and weir height. Similar data were obtained for H_2S absorption.

A computer program that incorporates the Murphree vapor tray efficiencies of H_2S and SO_2 and the reaction between these two components was written to solve the absorber operating problem. The column was assumed to be isothermal (a good assumption due to the small amount of H_2S being absorbed) and isobaric (a good assumption for columns at high pressure). Mass balance and equilibrium equations were written for each stage, and the resulting system of equations was solved by the multivariate Newton-Raphson technique. The column temperature and pressure, number of stages, feed flows and compositions, component tray efficiencies, reaction rate constant and tray volume must be specified. This model will be modified as experimental data for reactive absorption are obtained.

The crystallizer is being modified to accept separate feeds of dissolved H_2S and SO_2. Sulfur will be produced by chemical reaction. The absorption of H_2S enhanced by the presence of SO_2 in the solvent will be studied and the results used to develop a model that incorporates previous work on reaction kinetics.

PUBLICATIONS

1. Sciamanna SF, Lynn S. Sulfur solubility in pure and mixed organic solvents. *I & EC Research* 1988; 27:485.
2. Sciamanna SF, Lynn S. Solubility of hydrogen sulfide, sulfur dioxide, carbon dioxide, propane and n-butane in polyglycol ethers. *I & EC Research* 1988; 27:492.
3. Sciamanna SF, Lynn S. An integrated process for simultaneous desulfurization, dehydration, and recovery of hydrocarbon liquids from natural gas streams. *I & EC Research* 1988; 27:500.

Organometallic Synthesis and Catalysis Studies*

The Organometallic Chemistry Group focuses on two areas of research: *a)* reactions of polynuclear heteroaromatic nitrogen (PHN) compounds with organorhodium and organoruthenium complexes as well as catalysis studies on the regioselective hydrogenation of PHN compounds with the above-mentioned complexes as homogeneous catalysts; *b)* biomimetic catalysis directed toward the synthesis and catalytic activity of mimics of monooxygenase enzymes. The conversion of small hydrocarbons to their respective alcohols (*e.g.*, methane to methanol) is the major goal of this project.

BONDING OF POLYNUCLEAR HETEROAROMATIC NITROGEN LIGANDS TO (PENTAMETHYLCYCLOPENTADIENYL)RHODIUM DICATION: THE ROLE OF NITROGEN VERSUS π-COMPLEXATION ON THE REGIOSELECTIVE HYDROGENATION OF THE NITROGEN RING*

R.H. Fish, H-S. Kim, J.E. Babin, and R.D. Adams

The reactions of quinoline **(1)**, isoquinoline **(2)**, 1,2,3,4-tetrahydroquinoline **(3)**, and 2-methylquinoline **(4)** with (pentamethylcyclo- pentadienyl)rhodium dication [$Cp^*Rh(acetone)_3^{2+}$, $Cp^*Rh(acetonitrile)_3^{2+}$, or $Cp^*Rh(p-xylene)^{2+}X_2$; X = PF_6 or BF_4] were studied to ascertain nitrogen (N) versus π-bonding. Ligands **1** and **2** were found to form N-bonded rhodium complexes, while ligand **3** preferred π-coordination (η^6). Ligand **4** was found to provide both π- and N-bonded complexes. A single-crystal x-ray structural analysis of a derivative of [$Cp^*Rh(quinoline)(acetonitrile)_2^{2+}$, $Cp^*Rh(quinoline)(\mu-hydroxo)]_2^{2+}$ verified the N-bonding of ligand **1** to the rhodium metal center. We also found that the abovementioned Cp^*Rh^{2+} synthetic precursors were excellent catalysts or catalyst precursors for the selective hydrogenation of **1**, **2**, and **4** to their corresponding tetrahydro derivatives. This latter result defines the important role of N-bonding for regioselective nitrogen ring reduction.[1]

*These studies was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy and the Electric Power Research Institute under Contract No. DE-AC03-76SF00098.

MODELING THE DINUCLEAR SITES OF IRON BIOMOLECULES: SYNTHESIS AND PROPERTIES OF $Fe_2O(OAc)_2Cl_2(bipy)_2$ AND ITS USE AS AN ALKANE ACTIVATION CATALYST

J.B. Vincent, J.C. Huffman, G. Christou, Q. Li, M.A. Nanny, D.N. Hendrikson, R.H. Fong, and R.H. Fish

The study of synthetic models containing the $[Fe_2(\mu-O)(\mu-O_2CR)_2]^{2+}$ core established in the oxygen carrier protein hemerythrin (Hr) has received additional impetus and importance with the realization that such units may also be present in other dinuclear iron biomolecules. These include the purple acid phosphatases (PAP), ribonucleotide reductases (RR), and methane monooxygenases (MMO). By using a variety of tridentate N-based ligands (L), synthetic materials of formulation $[Fe_2O(O_2CR)_2L_2]$ have been prepared, establishing the accessibility and stability of this unit outside a polypeptide environment. The tridentate ligands, however, block all terminal binding sites, precluding investigation of native substrate or substrate-analogue binding. Use of bidentate ligands to overcome this problem has led to dimerization of the $[Fe_2O(O_2CR)_2]^{2+}$ unit to yield products containing $[Fe_4O_2(O_2CR)_4]^{4+}$. However, we reported a procedure that uses 2,2'-bipyridine (bipy) to allow access to a $[Fe_2O(O_2CR)_2]^{2+}$ product; in addition, we described the structure, properties, and alkane activation reactivity of $Fe_2O(OAc)_2Cl_2(bipy)_2$, which possesses Cl^- ligands bound to the now-available sixth coordination sites.[2]

CARBON-HYDROGEN ACTIVATION CHEMISTRY: HYDROXYLATION OF C_2, C_3, AND $CycloC_6$ HYDROCARBONS BY MANGANESE CLUSTER CATALYSTS WITH A MONOOXYGEN TRANSFER REAGENT

R.H. Fish, R.H. Fong, J.B. Vincent, and G. Christou

The C-H bond activation of alkanes with homogeneous catalysts that mimic the active site of monooxygenase enzymes is currently an extremely important and intense area of research. Although considerable effort has been focused on mimics of cytochrome P450 (which has a metallo-porphyrin center as the active site) few examples have been reported on non-porphyrin complexes. The interest in non-porphyrin complexes as C-H activation catalysts coincides with recent reports on methane monooxygenase enzymes, which have tentatively been assigned, via EXAFS analysis, as having a μ-oxo diiron non-porphyrin active site.

The reported metallo-non-porphyrin C-H activation catalysts are predominantly mononuclear metal complexes, whereas two studies were directed towards metal clusters containing iron. We reported that a series of manganese clusters (Figure) originally synthesized as models for the photosynthetic water oxidation enzyme site in green plants are novel C-H activation catalysts for the hydroxylation of C_2, C_3, and cycloC_6 hydrocarbons in the presence of a monooxygen transfer reagent. To our knowledge, this is the first reported attempt to evaluate the C-H bond reactivity of small hydrocarbons using non-porphyrin metal clusters as catalysts.[3]

$Mn_3O(O_2CCH_3)_6(py)_3$	$[Mn_3O(O_2CCH_3)_6(py)_3](ClO_4)$
1	**2**
$Mn_4O_2(O_2CPh)_7(bipy)_2$	$[Mn_4O_2(O_2CPh)_7(bipy)_2](ClO_4)$
3	**4**

FIGURE. Manganese-cluster catalysts for hydroxylation of C_2, C_3, and cycloC_6 hydrocarbons.

REFERENCES

1. Fish RH, Kim H-S, Babin JE, Adams RD. Studies on the bonding of polynuclear heteroaromatic nitrogen ligands to pentamethylcyclopentadienylrhodium dication: the role of nitrogen versus π-complexation on the regioselective hydrogenation of the nitrogen ring, *Organometallics* 1988; 7:2250.
2. Vincent JB, Huffman JC, Christou G, Li Q, Nanny MA, Hendrickson DN, Fong RH, Fish RH. Modeling the dinuclear site of iron biomolecules: synthesis and properties of $Fe_2O(OAc)_2Cl_2(bipy)_2$ and its use as an alkane activation catalyst, *J Am Chem Soc* 1988; 110:6898.
3. Fish RH, Fong RH, Vincent JB, Christou G. Carbon-hydrogen activation chemistry: hydroxylation of C_2, C_3, and CycloC_6 hydrocarbons by manganese cluster catalysts with a monooxygen transfer reagent. *JCS Chem Commun* 1988 (in press).

Energy-Related Organic Compounds (EROC): A Microcomputer Information Database of Potential Pollutants*

C.G. Daughton and J.F. Thomas

A commercial-scale "synthetic fuels" industry (*e.g.*, coal gasification, shale oil production) would generate vast quantities of liquid and solid wastes comprising highly complex assemblages of organic compounds from numerous chemical classes. These compounds are the subject EROC (Energy-Related Organic Compounds), a menu-driven relational database for MS-DOS microcomputer retrieval of physicochemical/biological properties, process-stream occurrence, chemical nomenclature, and full bibliographic citation information for all referenced data.

When completed, EROC will comprise three integrated modules: BCS (Bibliographic Citation System), CPSS (Chemical Properties, Structures, and Synonyms), and PSCC (Process-Stream Chemical Characterization). The third module, PSCC, is in the initial stages of development. The first two modules have been completed and are designed to function also as stand-alone software applications.

BCS is an information management system for all aspects of bibliographic citation. No experience in database use or programming is required of the user. BCS is fully menu-driven for all aspects of data entry, editing, data retrieval and report generation. The structure of BCS is completely "normalized"; the number of fields has been minimized, and code "look-up" tables have been used where appropriate. All references are linked with the other modules via unique accession numbers. Version β-1.0[1] is currently available from Dr. Christian Daughton.

CPSS is a fully menu-driven information system that describes the chemistry of organic compounds found in waste materials. CPSS allows retrieval of information concerning molecular structures, reactions, physicochemi-

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Oil, Gas, and Shale Technology of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

cal properties, chemical names/synonyms, miscellaneous chemical information, and comprehensive chemical nomenclature. Each compound (current total 1700) is assigned a unique identification number for relational linking among the numerous data tables. CPSS contains a wide selection of physicochemical properties that would be of use in designing or implementing environmental fate models.

With CPSS, querying for particular chemical classes requires no knowledge of chemical structure. Instead, use is made of a comprehensive hierarchical menu system based on numerous attributes of chemical structure. Queries for practically limitless combinations of functional groups can be executed simply by selecting appropriate functional group names. Complex queries are made possible by the use of an iterative filter system.

CPSS contains an index of all alternative names for each compound. These include CAS, IUPAC, common, trivial, and trade names, and acronyms. Compounds can be queried on the basis of any of their names, roots, or approximations. The synonyms facility serves as a cross-referenced thesaurus of chemical names. Currently, for 1700 compounds there are 5784 synonyms.

CPSS nomenclature encompasses a broad spectrum of terminology that could potentially be of relevance to any of the other EROC modules. Representative classes of information include *a)* nearly all of the potentially relevant prefixes and suffixes in organic chemistry that comprise "substitutive nomenclature"; line structures and definitions are given for chemical radical names; *b)* common abbreviations and acronyms, especially those used in the fields of chemistry and the environment; *c)* information on the elements of the periodic table; *d)* units of measure; *e)* common and uncommon prefixes and suffixes; *f)* thorough listing and definition of chemical classes, including representative line structures; *g)* listing and line structures for all common aromatic and heteroatomic ring systems; and *h)* other related nomenclature for organic and analytical chemistry, chemical engineering, and toxicology.

Specific uses of EROC are numerous. Those that would have immediate utility include abstraction of information critical to pollution monitoring. For example, many geographical areas (especially in the western United States), could support commercial development of multiple types of industries for hydrocarbon extraction/conversion. Marker, or tracer, compounds will need to be identified so that the source of suspected pollution episodes can be inferred from monitoring data. The minimum number of types and the relative concentrations of the suite of compounds describing the unique "fingerprint" of a particular waste can be extracted from the EROC data base by means of factor analysis. Data on commonalities and unique qualities of different wastes would also be valuable for anticipating new water- and air-quality regulations that will probably evolve during construction of commercial-scale facilities; such regulations are likely because of the unique nature of the raw materials and processes that would be used by these industries.

Version β-1.0[2] of CPSS is currently available from Dr. Christian Daughton.

Other projects completed during FY 1988 include investigation of the importance of vapor-phase photochemistry in the environmental fate of nitrogen heterocycles that could be emitted to the atmosphere from the retorting of oil shale;[3] and development of a numeric model for removal of dissolved ammonia from wastewaters by use of a membrane separation technique that uses microporous polytetrafluoroethene tubes.[4]

PUBLICATIONS

1. Daughton CG, Langlois GW. BCS: Bibliographic Citation System data base, version β-1.0-22 (for MS-DOS systems), Lawrence Berkeley Laboratory, 1988.
2. Daughton CG, Langlois GW. CPSS: Chemical Properties, Structures, and Synonyms data base, version β-1.0-88, Lawrence Berkeley Laboratory, 1988.
3. Blatchley ER III. Atmospheric chemistry of expected nitrogen heterocycle emissions from oil shale operations. *Ph.D. thesis*, University of California Berkeley, Department of Civil Engineering, 1988.
4. Sakaji RH. Removal of ammonia from oil shale process waters using a tubular microporous polytetrafluoroethene membrane. *Ph.D. thesis*, University of California Berkeley, Department of Civil Engineering, 1988.

Studies of Animal Cell Cultures in Hollow-Fiber Reactors*

E. Fernandez, A. Mancuso, D. Clark, and H. Blanch

Normally, observations of extracellular reactor conditions allow only indirect understanding of the catalytic processes occurring inside the cell. To observe the intracellular environment directly, we have applied nuclear magnetic resonance (NMR) spectroscopy. This technique is particularly appealing because it is noninvasive, involving only static magnetic fields and radio waves. A hollow-fiber culture system/NMR probe combination has been developed which is compatible with commercially available spectrometers. This permits observation of phosphorylated and carbonaceous metabolites inside hybridoma cells.

NMR has two disadvantages relevant to studies of mammalian cells. First, it is relatively insensitive when compared to other analytical methods. As a result, previous investigators have used NMR spectroscopy to study cells at high densities to maximize the signal-to-noise ratio obtained. Second, commercial NMR sample probe

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution, Energy Storage Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

geometries restrict the amount of apparatus that can be used to support a cellular sample. Consequently, mass transfer of nutrients and waste products has been poor, and the samples under study have generally only been stable for a few hours at a time. While such a system can provide useful qualitative metabolic information, we have been interested in exploiting the quantitative nature of NMR in steady-state and transient studies of animal cell metabolism. Our goals, therefore, have been to develop an apparatus that maintains hybridoma cells at the high densities necessary for NMR experiments and provides adequate mass transfer for nutrients and waste products, allowing us to study a stable culture for days or weeks.

We have chosen the hollow-fiber bioreactor (HFBR) for these studies because it can provide high cell densities (near those found in animal tissue) and has good mass-transfer characteristics. The culture system is designed for long-term operation, including stable temperature control ($< 0.1°C$), and has conventional probes for dissolved oxygen and pH. Dissolved oxygen and pH control are accomplished manually by mixing CO_2, N_2, and O_2. Because environmental control has been a high priority, we have abandoned use of commercial NMR probes and designed and constructed our own probes to permit greater flexibility in the design of the culture system.

The most important part of NMR probes is generally the rf coil, or "antenna," used to irradiate the sample with radio waves and receive the subsequent emitted signal. The coil must be capable of handling the high voltages used in transmission (100 V or more for short periods) and sensitive enough to detect the small voltages induced in the coil by the sample after irradiation (on the order of microvolts). In addition, to maximize the signal-to-noise ratio, we have been interested in increasing the size of the sample. We have evaluated three different coil designs for this application: the solenoid, the loop gap resonator (LGR), and the slotted tube resonator (STR). Of these, only the STR is aligned coaxially with the cylindrical NMR probe and the homogeneous portion of the static magnetic field. Thus, although we found the other two coil designs to be more sensitive (30-40% per unit volume at 15 ml), we chose the STR for reasons of convenience.

Based on these test data, we have designed and constructed NMR probes for single-resonance ^{13}C and ^{31}P NMR experiments at 9.4 tesla. We have also constructed a tunable probe capable of both ^{13}C and ^{31}P NMR. A coil tuned for the ^{1}H frequency was also included in the tunable probe to facilitate optimization of the static magnetic field based on the signal from water in the sample.

By mounting the HFBR inside this last probe, we have been able to observe phosphorylated metabolites in hybridoma cells online. To date, we have examined the cells under three different conditions: *a)* during an interruption of medium flow (effectively a rapid starvation of oxygen); *b)* before, during, and after a glucose step change; and *c)* over several hours, under varied oxygen levels. Examination of these NMR data suggests that most energy in these cells is derived from oxidative phosphorylation rather than from glycolysis.

We have also performed a preliminary steady-state ^{13}C NMR experiment in which the glucose in the feed was changed from naturally abundant glucose to glucose labeled with ^{13}C in the C-1 position. This experiment showed lactate, alanine, and some unidentified compounds.

Future research topics are examined in the following paragraphs.

CONTINUOUS MEASUREMENT OF P:O RATIO

To measure an apparent P:O ratio, we plan to use NMR techniques to measure the rate of ATP hydrolysis and/or formation and conventional methods to measure the oxygen uptake rate. If the cells are deriving most of their energy from oxidative phosphorylation, this number should be near three. Anything over this number would represent a significant contribution to energy production by other pathways (*e.g.*, glycolysis).

MEASUREMENT OF GLYCOLYTIC RATE

By performing ^{13}C NMR experiments involving ^{13}C-labeled glucose, we expect to obtain a glycolytic rate by monitoring lactate production from glucose as well as glucose consumption rate. This data would complement measurement of the P:O ratio.

STEADY-STATE ^{13}C EXPERIMENTS

We would like to examine the relationship between glutamine, glucose, and oxygen by performing experiments utilizing ^{13}C-labeled glutamine or glucose to monitor the formation of intermediates and products of their metabolism under different concentration ranges of these nutrients. We are interested in examining the dependence of energy production, waste product formation, and antibody formation under various conditions.

Separations by Reversible Chemical Association*

C.J. King, A.S. Kertes, J. Tamada, D. Arenson, A. Garcia, L. Poole, J. Starr, W. Rixey, and M. Ng

Reversible chemical association, or complexation, is an attractive method for recovery of carboxylic acids, alcohols, glycols and related substances from the dilute solutions resulting from manufacture by fermentation of biomass. We have focused upon extraction and sorption processes.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Systems Research, Energy Conversion and Utilization Technologies (ECUT) Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

EXTRACTION OF CARBOXYLIC ACIDS

We have measured equilibria for extraction of acetic, succinic, malonic, lactic, maleic and fumaric acids from aqueous solution by Alamine 336 (Henkel Corp.; tri-C8 to C10 amine) in several diluents, including heptane, methyl isobutyl ketone (MiBK), chloroform, methylene chloride, and nitrobenzene. The association constant for the complex depends upon the acidity of the acid and the chemical nature of the diluent. Tendencies for overloading (more than one acid extracted per amine) are also strongly affected by the chemical nature of the diluent. In light of spectroscopic measurements and comparable results from prior studies, we have interpreted our results through mass-action-law modeling. We have obtained and interpreted exploratory data underlying regeneration of amine extracts by four different methods: *a)* back-extraction into water following a change in temperature; *b)* back-extraction into water following a change in diluent composition (can be combined with *a*); *c)* precipitation of a low-solubility acid (*e.g.*, fumaric) following evaporation of diluent and/or temperature change; *d)* back-extraction into an aqueous solution of a volatile tertiary amine, followed by concentration and decomposition of the trialkylammonium carboxylate to produce the product acid and the light amine for recycling.

Future research will explore more deeply the various methods of regeneration and will investigate alcohol and phenol diluents and competitive equilibria in the presence of multiple acids.

SORPTION OF CARBOXYLIC ACIDS

We have used various functionalized basic polymeric sorbents to measure and interpret equilibria for uptakes of acetic acid and water from aqueous solution. We have also measured and interpreted equilibria for leaching of sorbed acetic acid by solvents having various degrees of basicity. Most basic sorbents are difficult to regenerate; however, we have demonstrated the feasibilities of regenerating Dowex MWA-1 tertiary amine resin (Dow Chemical Co.) by hot-air stripping, regenerating Aurozez polybenzimidazole resin (Celanese Chemical Co.) by leaching with successively less polar solvents, and regenerating polyvinylpyridine sorbents by leaching with common solvents.

EXTRACTION OF ALCOHOLS AND GLYCOLS

We have found that phenols interact more strongly with alcohols than do other common solvents. In studies of extraction of ethanol and the four butanol isomers by m-cresol in various diluents, we have shown that specific 1:1 alcohol:cresol complexes are formed.

Future research will address extraction of glycols, use of sorbents with phenolic groups, other functional groups effective for complexing of alcohols and phenols, and the possibility of recovery of glycols through adductive crystallization.

NON-WET ADSORBENTS

Sufficiently non-polar polymeric adsorbents, such as styrene-divinylbenzene and pyrolyzed sulfonated styrene-divinylbenzene copolymers, are not wetted by dilute aqueous solutions. In the non-wet state, such adsorbents take up solutes of moderate and high volatility at substantial rates. They provide advantages of low concomitant water uptake and an ability to fractionate among solutes on the basis of volatility. Measurements of adsorption of acetic and propionic acids, ethanol, and 1,3-butanediol have demonstrated that the rate limit is Knudsen diffusion through pores, and that performance of fixed-bed adsorbers can be rationalized through that concept.

Future work will explore the use of these non-wet adsorbents at higher temperatures, which should give economically attractive uptake rates for glycols.

Ultrasensitive Laser Spectroscopy*

R.E. Russo, J.D. Spear, and R.J. Silva

Photothermal laser spectroscopic techniques were developed for ultrasensitive optical absorption measurements of rare-earth and actinide solutions. The techniques developed and compared in FY88 were photothermal deflection (PDS) and thermal lensing (TLS) spectroscopies. For PDS and TLS, we investigated using modulated continuous-wave (cw) and pulsed laser excitation sources.

Optical absorption by the modulated or pulsed excitation laser and subsequent non-radiative relaxation (heating) induce a refractive index gradient in the sample solution. For TLS, a probe laser propagating collinear to the excitation laser will be defocused by the induced refractive index gradient. A pinhole and photodiode are used to measure the change in probe-beam intensity due to defocusing, which is related to the optical absorption. For PDS, the excitation and probe beams cross. The refractive index gradient causes a deflection of the probe beam. A lateral position sensor measures the deflection, the magnitude of which is related to the sample's absorption coefficient. PDS probes the maximum gradient of the refractive index whereas TLS probes its curvature.

For FY 1988 cw work at LBL, we employed an argon-ion pumped dye laser, using rhodamine 6G dye to excite the 575 nm transition of N^{3+} (molar absorptivity = 6.9 L/mole cm). We developed a dual-beam differential arrangement for both the PDS and TLS systems. Dye laser power normally used was 50 mW at 575 nm. Using both cw PDS and TLS, we can regularly measure Nd

*This work was performed under the Lawrence Livermore National Laboratory Contract No. W-7405-ENG-48 for the U.S. Department of Energy.

† Nuclear Chemistry Division, Lawrence Livermore National Laboratory.

down to 3 x 10^{-6} molar. The signal-to-noise ratio at this concentration is ~10 for PDS and 18 for TLS. The TLS system appears to be slightly more sensitive, although further work is needed to optimize both systems and obtain an accurate comparison.

At LLNL, both PDS and TLS were developed using the pulsed Nd:YAG pumped dye laser. For Nd^{3+} (at λ = 521 nm, molar absorptivity = 4.7 L/mole cm), we measured a concentration of 3 x 10^{-6} M in 0.001 M HCl, with a signal-to-noise ratio of ~65. The detection limit (S/N = 3) is therefore calculated to be 1.4 x 10^{-7} M. This detection limit is the best obtained for any of our techniques, including photoacoustic spectroscopy (PAS). In addition, the PDS detection limit reported above was obtained using only 0.75 mJ/pulse, compared to the 2 mJ/pulse normally employed for PAS. Therefore, the absorptivity (cm^{-1}) for Nd using pulsed PDS (1 mJ/pulse) would be ~4 x 10^{-7}, a better value than those reported in the literature for comparable techniques. A lower pulse energy was required using PDS and TLS because the beam is tightly focused, compared to PAS, and the resultant high power density causes ablation of the sample cell. Also, the PDS data seem to be affected by long-term drift. We can average longer with the PDS and TLS techniques, compared to PAS, but the spectrum becomes influenced by long-term drift. At this time, it is not known where the drift originates.

We have preliminary results for pulsed TLS. Although we can easily measure 1 x 10^{-5} M, the spectrum is strongly influenced by the spectrum of the dye laser itself. In TLS, the excitation and probe beams overlap (collinear). A bandpass filter is used to pass the HeNe laser to the photodiode but not the excitation dye laser. However, because of the high peak power of the dye laser, a small amount of excitation light leaks through the filter and is measured by the photodiode. A more effective filter or use of a crossing configuration would permit an accurate detection limit for Nd using pulsed TLS.

During FY 1989, the sensitivity of TLS will be improved by using a better blocking filter to eliminate the excitation wavelength from the detector photodiode. These photothermal techniques will be employed to measure complexation constants for actinides in various aqueous solutions.

REFERENCE

1. Spear JD, Russo RE, and Silva RJ. *Applied Spectroscopy* 1988; 42:1103-05.

Pulsed Laser Ablation for Thin-Film High-Temperature Superconductors*

R. Russo and B. Olsen†

This project involved study and development of pulsed laser ablation for making thin-film high-temperature superconductors. Laser ablation involves non-thermodynamic, shock-wave processes that occur from the interaction of a short-pulsed, high-energy laser focused on a solid material surface. Material with the exact stoichiometry as the target can be removed. The ablated material is collected on a substrate placed in close proximity to the ablation plume. We have used this technology to produce superconducting thin films of $YBa_2Cu_3O_{7-\gamma}$.

During FY 1988, a pulsed laser ablation system was designed and constructed as a joint effort between the Lawrence Berkeley Laboratory (LBL) and the Lawrence Livermore National Laboratory (LLNL). The system is housed at LLNL because of the availability of an excimer laser. A vacuum chamber was constructed containing several feedthroughs, a filament heater, and optical ports. The chamber accommodates four separate bulk targets and substrates simultaneously. With these capabilities, we can deposit multilayered films from different materials and can deposit several films consecutively without exposing the chamber to the environment.

A pulsed high-energy excimer laser was used because its characteristic ultraviolet wavelength contributes to a photophysical interaction with less thermal evaporation involved in the material removal processes than would be the case using infrared lasers. The laser can deliver up to 1.5 J per pulse at 308 nm. We use 750 mJ per pulse and lightly focus the beam to obtain 1.5 J/cm^2 energy density on the targets. Strontium titanate substrates, placed 1.5 cm from the bulk target, were used to collect the ablated vapor. With these conditions, we achieved a deposition rate of ~5 Å per pulse (repetition rate of one pulse per second). The laser ablation approach maintains excellent control of the material's stoichiometry with these condi-

*This work was supported by Assistant Secretary of Conservation and Renewable Energy, Office of Energy Storage and Distribution, Energy Storage Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

†Chemistry and Materials Division, Lawrence Livermore National Laboratory

tions; the elemental composition ratio in the film matched that in the bulk target. Analytical techniques of x-ray fluorescence, Auger spectroscopy, Rutherford spectroscopy, and atomic emission spectroscopy were used to compare the elemental composition ratio of the bulk and thin-film samples.

The figure shows resistance *vs* temperature for one of our YBCO films. The film is ~2 μm thick on a 5 x 5 mm^2 strontium titanate substrate. The film was annealed over a ten-hour period with a maximum temperature of 850°C. The onset of superconductivity occurred at 92°K with zero resistance reached at 72°K. Resistance was measured with a standard four-point probe technique.

During FY 1989, an improved laser ablation system will be constructed at LBL. This system will provide the capability for depositing multi-layered, thin-film configurations and for depositing films in a reactive, secondary plasma environment. We plan to deposit superconducting films from materials containing bismuth and thallium, and to produce films that are superconducting as deposited, *i.e.*, without post annealing.

Interactions with industry will be initiated to determine their needs in this field and to explore possible collaborative efforts.

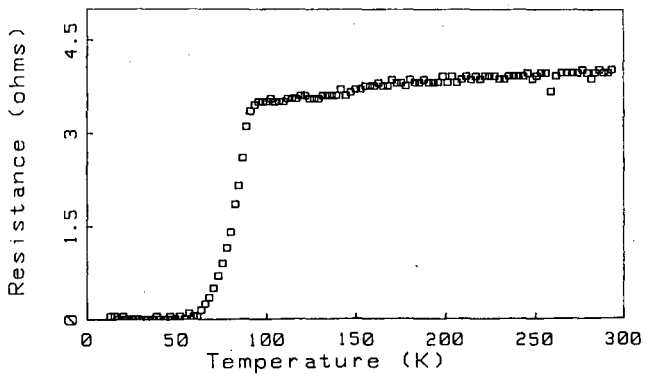


FIGURE. Plot of resistance *vs* temperature for a YBCO film. The film is ~2 μm thick on a 5 x 5 mm^2 strontium titanate substrate. The film was annealed over a ten-hour period with a maximum temperature of 850°C. The onset of superconductivity occurred at 92°K, with zero resistance reached at 72°K. The resistance was measured using a standard four-point probe technique (XBL 8812-4093).

ENVIRONMENTAL RESEARCH PROGRAM STAFF

Tihomir Novakov, Program Leader
Nancy Brown, Deputy Program Leader

Susan Anderson*
Frank Asaro†
Henry Benner
Charles Blanchard
Nancy Brown†
Shih-Ger Chang†
Robert Cheng
Peck Cho‡
Mariah Cochrane
John Dailey
Raymond Dod
Cheryl Ehorn
Ofodike Ezekoye
David Faris
Luis Feliu
Carlos Fernandez-Pello
Charles Fleischman
Stephanie Frolich
Ian Fry
Robert Giauque
Gloria Gill
Iskander Gokalp*
Philippe Goix
Ralph Greif
Yogesh Gubbi
Lara Gundel
Anthony Hansen
John Harte
Erika Hoffman
Kenneth Hom
Wei-Ming Huang
Gary Hubbard
Margaret Huflejt
Frank Hurlbut
Kristine Ing
Liwen Kao
Arthur Li
David Littlejohn
David Liu
Jau-Huai Lu
Donald Lucas
John Maguire
Julieta Marcelino
Samuel Markowitz
Richard Martin
Andrew Maxson
Rolf Mehlhorn
Harvey Michaels
Helen Michel
Aliza Mizrahi*
Katherine Moore
Fred Mowrer
Amos Newton
Tihomir Novakov†
Bo Ogorevc*
Antoni Oppenheim
Roland Otto
Lester Packer†
Isadore Perlman
Ahmed Rashed
Chang Woo Rhee
Frank Robben
Eva Robinson
Robert Sawyer
Frank Schipperijn
Richard Schmidt
Birger Schmitz*
Richard Schneider
Di-Xiu Shen*
Ian Shepherd§
Linda Sindelar
Gordon Stevens
Horton Stewart§
Fred Stross*
Lawrence Talbot
Louie Tobias*
Eric Wakahiro
Yizhong Wang*
R. Brady Williamson
Linda Wroth
Feng-Hua Yang
Xun Xu

*Participating Guest
†Group Leader
‡University of California Davis
§University of California Berkeley

ENVIRONMENTAL RESEARCH PROGRAM

INTRODUCTION

The principal objective of the Environmental Research Program is to understand the formation, transformation, transport, and effects of energy-related pollutants on the environment, and how these are influenced by energy generation and emission control technology. Some of the ongoing projects and those that will be initiated in the near future address topics with the general framework of global environmental change. Others deal with studies necessary to understand the fundamentals of generation and effects of environmental contaminants. This multidisciplinary research program includes fundamental and applied research in physics, chemistry, engineering, and biology, as well as research on the development of advanced methods of measurement and analysis. The Program's Annual Report contains summaries of research performed during FY 1988 in the areas of atmospheric aerosols, flue gas chemistry, combustion, membrane bioenergetics, and analytical chemistry.

The main research interests of the Atmospheric Aerosol Research Group concern the chemical and physical processes that occur in haze, clouds, and fogs, and development of novel methods for individual particle characterization.

The Flue Gas Chemistry Research Group is engaged in research whose aim is to help develop new processes for simultaneous SO_2 and NO_x removal.

The Combustion Research Group studies complex combustion processes by acquiring a fundamental understanding of the physical and chemical processes that determine the combustion efficiency, formation, and emissions of species from these processes.

The Membrane Bioenergetics Group studies the effects of strongly chemically reactive compounds generated within cells.

The main emphases in Analytical Chemistry have continued to be in the area of asteroid impacts and mass extinctions.

The short reports that follow describe the program activities in FY 1988. For many of these reports, more detailed papers have been or will be published in appropriate scientific journals.

ATMOSPHERIC AEROSOLS

Cloud Nucleation Characteristics of Smokes from Different Fuels*

A.D.A. Hansen and T. Novakov

Smoke particles from the burning of fuels were historically considered to be hydrophobic; in the more recent past, it was believed that the presence of soluble species (e.g., sulfates) could modify the surface characteristics to make smoke particles more able to act as nuclei for the formation of fog or cloud droplets. However, laboratory measurements of smoke particle incorporation into cloud droplets in condensing plumes had not been widely performed.

In this work, we used our mixing-type cloud chamber to study the behavior of smokes from different fuels and to study the effect of fuel sulfur content on their droplet nucleation characteristics. We burned several liquid fuels (diesel fuel, kerosene, JP-4 jet fuel, Alaskan and Californian crude oils), as well as small fir wood cribs. In some experiments, we added thiophene to the JP-4 to increase its sulfur content. The results showed that the fraction of the mass of smoke incorporated into cloud droplets (under fixed cloud chamber conditions) varied considerably from fuel to fuel, did not bear any relationship to either the fuel sulfur content or the sulfate content of the resultant smoke, and instead depended on combustion efficiency and heat release per unit of fuel consumed. The greater the heat release (progressing, for example, from diesel fuel to jet fuel), the smaller the mass fraction of the smoke incorporated into cloud droplets.

This result suggests that combustion dynamics—and not chemical composition of fuel or smoke—plays a major role in determining water nucleation of smoke particles via their surface characteristics. This result also has implications for assessing the impact of combustion emissions on global climate change.

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Physical and Technological Research Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by Lawrence Livermore National Laboratory.

Acceleration of Submicron-Sized Particles*

W.H. Benner and R. Otto

We have continued to develop a technique that will eventually be used to determine the elemental composition of individual particles in real time. Three separately constructed components—source of charged particle, a device producing particle beams, and an electrostatic particle accelerator—were coupled and extensively tested as a way to produce particles traveling at ~1 km/sec. In this combined system, NaCl particles having +1 unit of charge and diameters of 0.02, 0.05, or 0.2 μm were generated in the particle source. These particles were then drawn through a differentially pumped skimmer system (particle-beam production), and the resultant beam of particles that traveled at sonic velocity in vacuum served as a way to inject the charged NaCl particles into the electrostatic accelerator. In the electrostatic accelerator, the particles were accelerated through six successively increasing voltage stages with a terminal target voltage of -125 kV. Theoretically, this acceleration produced particles having the velocities 2.4 km/sec, 0.8 km/sec, 0.4 km/sec for particles 0.02 μm, 0.05 μm, and 0.2 μm in diameter, respectively. These stated velocities include a preacceleration velocity of 0.3 km/sec generated by the particle beam system.

After alignment of the components, the system was tested by impacting accelerated particles onto Al and Au targets. Examined by electron microscopy, the targets showed that the impacts produced shallow, smooth-rimmed craters. Some craters contained residue of the impacting particle. These observations indicate that impacts melted most of the NaCl particle but were probably not energetic enough to ionize the particulate material. Our approach for developing a way to ionize particles and determine their composition by mass spectrometry appears feasible, however, because more energetic impacts can be produced by increasing the particle charge and acceleration voltage.

We have begun constructing a particle source that produces test particles of much greater charge. By charging solution droplets as they form and evaporating the solvent, we will produce residual solute particles charged to the Rayleigh limit Theoretically, 0.02-μm, 0.05-μm, or 0.2-μm particles charged to the Rayleigh limit and accelerated through 125 kV will have velocities of 16.8,

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Physical and Technological Research Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

10.7, or 5.2 km/sec, respectively. Particle impacts at these velocities are expected to ionize the particulate components.

NO_2 and SO_2 Reactions on Cold Surfaces*

W.H. Benner, A. Mizrahi, and T. Novakov

Formation of nitrate and sulfate on terrestrial surfaces leads to acidification of the surface because of the accompanying formation of hydrogen ion. The reaction between NO_2^- ion and S(IV) ion in aqueous solution has been studied extensively; much less attention has been paid to reactions on cold surfaces such as ice crystals and frost-covered surfaces.

A chillable glass finger was positioned inside a glass flask that could be charged with several torr of $H_2O(v)$, $NO_2(g)$, $SO_2(g)$ and then filled to atmospheric pressure with clean air. The finger temperature was reduced during several minutes of chilling to produce surface temperatures between room temperature and -45°C. This temperature (reaction temperature) was maintained for 20 min, after which it was rinsed with water. NO_2^-, NO_3^-, S(IV), and $SO_4^=$ were determined in the rinse water by ion chromatography.

The formation of NO_2^- and NO_3^- were observed when the surface was exposed to NO_2 and $H_2O(v)$. The ratio of NO_3^-/NO_2^-, always much greater than 1, was not as expected from the disproportionation of NO_2 in H_2O, where the ratio is 1. The formation of S(IV) and $SO_4^=$ was observed when SO_2 and $H_2O(v)$ were present. When mixtures of NO_2, SO_2, and $H_2O(v)$ were present in the flask, $SO_4^=$ increased and neither NO_2^- nor S(IV) was detected. The general pattern of SO_4^- and NO_3^- formation with respect to reaction temperature was that product increased from a negligible amount at room temperature to a maximum between 10° and -10°C and then decreased to about 50% of the maximum at temperatures below -10°C. The influence of acid catalysis on the product yield was tested by the addition of HCl(g) into the reaction system. Its presence did not appear to change product yield, but maximum sulfate production was shifted to slightly lower temperature.

The reaction between NO_2^- and S(IV) in water primarily produces hydroxylamine disulfonic acid and hydroxylamine monosulfonic acid, but these cannot be hydrolyzed to $SO_4^=$ in the time period of our experiments. Therefore, the observation of $SO_4^=$ formation on the chilled finger suggests that a different reaction occurs, and the oxidation via adsorbed NO_2 is probable. Also, the observed formation of only relatively small amounts of NO_2^- in the absence of SO_2 suggests that the disproportionation of NO_2 in water is affected by physical reaction conditions.

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Physical and Technological Research Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Sulfate Formation by Reaction of SO_2 with NH_3*

W.H. Benner, B. Ogorevc, and T. Novakov

The absorption of SO_2 into atmospheric droplets provides a reaction medium in which oxidants such as H_2O_2 and O_3, or particle surfaces, can convert SO_2 to $SO_4^=$. The role of NH_3 in this system is that of a buffer and a cation to help maintain ionic charge balance. In the gas phase, SO_2 and NH_3 are known to react to produce many oxysulfur products. This gas-phase reaction has been suggested as a source of particulate $SO_4^=$ in the atmosphere but has received little investigative focus. Previous studies examined the types of products formed but not the fractional yield of each product.

A flow system was designed in which 1-100 ppm of each gas in air could be mixed, drawn through a glass reactor, and then bubbled into water. The water vapor content of the gases could also be adjusted from about 1% to 70% relative humidity. After drawing the mixed gases through the system, the reactor was flushed with air and then rinsed with water. The reactor rinse water and the bubbler water were analyzed for $SO_3^=$ and $SO_4^=$ by ion chromatography.

When only SO_2 was drawn through the system, regardless of RH (relative humidity), >95% of the collected sulfur was found in the bubbler; of this percent, >95% was in the form of S(IV). (A small amount of sulfate was found in both the reactor and bubbler.) When equal concentrations (v/v) of SO_2 and NH_3 were drawn through the system, sulfate was observed to form in the reactor but not in the bubbler. Sulfate formation was dependent on the RH, $[SO_2]$, and $[NH_3]$. At 70% RH and 30 ppm of SO_2 and NH_3, as much as 50% of the total SO_2 sampled through the system was oxidized to sulfate. Of the sulfate formed, 95% was always found in the reactor tube. At 30 ppm of each gas and 4% RH, negligible formation of sulfate, when expressed as a percent of the SO_2 drawn through the system, could be attributed to the presence of NH_3. However, when the gas concentrations were reduced to ~1 ppm each, a large percentage of the SO_2 was oxidized to sulfate in the reactor tube.

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Physical and Technological Research Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the National Science Foundation under Contract ATM 8713712.

Five findings related to sulfate formation in this reaction system were determined from this work: 1) water vapor is required for the oxidation; 2) the composition of the reactor tube surface influenced sulfate formation — fractional conversion on surfaces increased on the order Teflon < glass < stainless steel; 3) in glass reactors of equal volume, fractional conversion increased as the surface/volume ratio of the reactor tube increased; 4) the

Removal of NO from Flue Gas by Tetrasulfophthalocyanine Complexes of Iron (II) and Cobalt (II)

D.K. Liu, G. Stevens, and S.G. Chang

We have synthesized water-soluble tetrasulfophthalocyanine (TSPc) complexes of iron (III), iron (II), and cobalt (II) according to the procedure of Weber and Busch.[1] The Fe(II)TSPc complex was prepared by using sodium dithionite to reduce Fe(III)TSPc. These metal TSPc complexes have been characterized by elemental analysis as well as by UV-visible and mass spectroscopic techniques. We have demonstrated by UV-visible spectroscopy that the TSPc complexes of Fe(II) and Co(II) can bind nitric oxide to form nitrosyl adducts. Furthermore, we have shown that aqueous solutions of both Fe(II)TSPc and Co(II)TSPc are capable of removing NO from a simulated flue gas mixture containing ~550 ppm NO and variable amounts of O_2 in a wet scrubber system maintained at 55°C. In the case of Co(II)TSPc, the NO absorption reaction was more effective at higher O_2 content. At pH 7, the stoichiometric ratio NO/Co was 0.23, 0.25, and 0.41 at 0%, 5% and 20% O_2, respectively. At pH 3 and 5% O_2, NO/Co was 0.18. Ion chromatographic analyses of the scrubbing liquor showed that ~34% of the absorbed NO was converted to NO_3^-. Purging the scrubbing liquor with O_2 or heating it to ~80°C for 5 h resulted in the recovery of more NO_3^-, with up to ~80% of the NO absorbed accounted for by NO_3^- formation. In the case of Fe(II)TSPc, a NO/Fe ratio of 0.59 was obtained at pH 4.2 with 5% O_2 in the flue gas.

REFERENCES

1. Weber JH, Busch, DH. Complexes derived from strong field ligands. XIX. Magnetic properties of transition metal derivatives of 4,4',4'',4'''-tetrasulfophthalocyanine. *Inorg Chem* 1965; 4:469.

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburgh Energy Technology Center, Pittsburgh, PA.

Removal of Nitrogen and Sulfur Oxides from Flue Gas Using Aqueous Emulsions of Yellow Phosphorus and Alkali

D.K. Liu and S.G. Chang

We have successfully demonstrated that an aqueous emulsion containing molten yellow phosphorus (P_4; m.p. = 44.1°C) and an alkali such as limestone ($CaCO_3$) can be used for simultaneous removal of NO_x and SO_2 from a simulated flue gas mixture in a wet scrubber. The reaction was carried out at 55°C in a jacketed reactor containing 0.9 *l* of a P_4 (3.3% w/w)/$CaCO_3$ (5.0% w/w) slurry at pH 7.5. The flue gas mixture was composed of 560 ppm NO, 2900 ppm SO_2, 10% O_2, and the balance was N_2. A $CaCO_3$ absorber was placed downstream to capture both P_4- and NO-derived products. As shown in the Figure, ~95% of the NO and all of the SO_2 in the flue gas could be removed for at least 3 h. The solid collected from the scrubber after the reaction was shown by laser Raman spectroscopy to contain $CaSO_4 \cdot 2H_2O$ in addition to

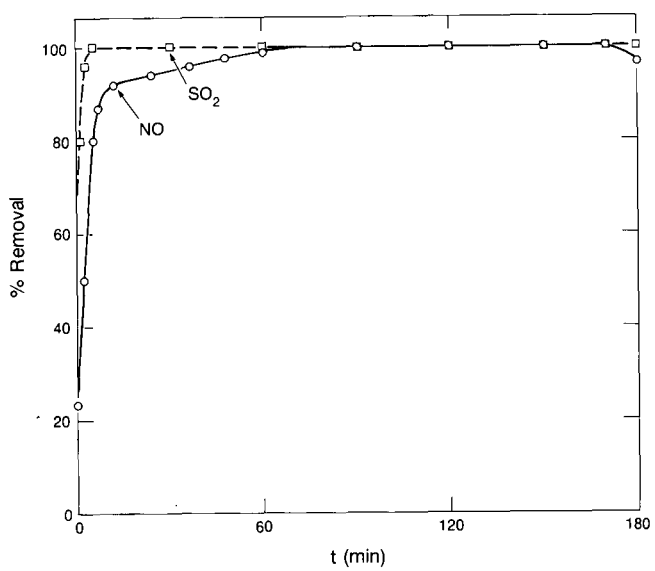


Figure. Simultaneous NO and SO_2 removal from flue gas using a molten yellow phosphorus/limestone slurry. (XBL 886-9664)

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburgh Energy Technology Center, Pittsburgh, PA.

unreacted $CaCO_3$ and P_4. The liquid phase in both the scrubber and the absorber was analyzed by ion chromatography, revealing the presence of that NO_2^-, NO_3^-, $SO_3^=$, $SO_4^=$, $H_2PO_2^-$, $HPO_3^=$, and $HPO_4^=$. Furthermore, we found that ~40% of the NO absorbed ended up as hydroxylamine disulfonate (HADS) and amine disulfonate (ADS) in scrubbing liquor, both compounds were subsequently hydrolyzed to NH_4^+. Therefore, the use of yellow phosphorus and an alkali for combined NO_x and SO_2 removal could result in production of valuable fertilizer materials, including ammonium nitrate and phosphate.

A Study of the Hydrolysis of Disulfate Ion

Di-Xen Shen, David Littlejohn, and Shih-Ger Chang

In an earlier study of the oxidation of bisulfite ion, we discovered that the oxidation reaction proceeds via an intermediate, determined to be disulfate ion, which then hydrolyzes to form sulfate ions and hydrogen ions. Other researchers had found that the rate of hydrolysis was influenced by other ions in solution. We have systematically investigated the effect of ions found in scrubbing solutions on the hydrolysis of disulfate ion.

The disulfate salt was mixed with a solution of the ion under study, and the reaction was monitored by two techniques. Raman spectrometry permitted observation of the decay of the disulfate ion and the growth of sulfate and bisulfate ions. However, the low concentrations often used in the study yielded weak signals, making accurate determination of the rate difficult. Use of a recording pH meter with a fast-response pH probe to record the change in pH of the solution proved to be simpler and more accurate than Raman spectrometry. This method was used for most measurements.

A number of cations and anions have been studied. Magnesium and calcium ions, often found in scrubbing solutions, greatly increased the hydrolysis rate. Of the anions studied, sulfite and thiosulfate were found to produce the largest hydrolysis rate increases. The results are shown in the Figure, where the observed rate constant for disulfate hydrolysis at 20°C is displayed for the ions studied. We are currently studying the influence of other ions on disulfate ion hydrolysis. These results will allow calculation of the lifetime of disulfate ion in scrubbing solutions.

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburgh Energy Technology Center, Pittsburgh, PA.

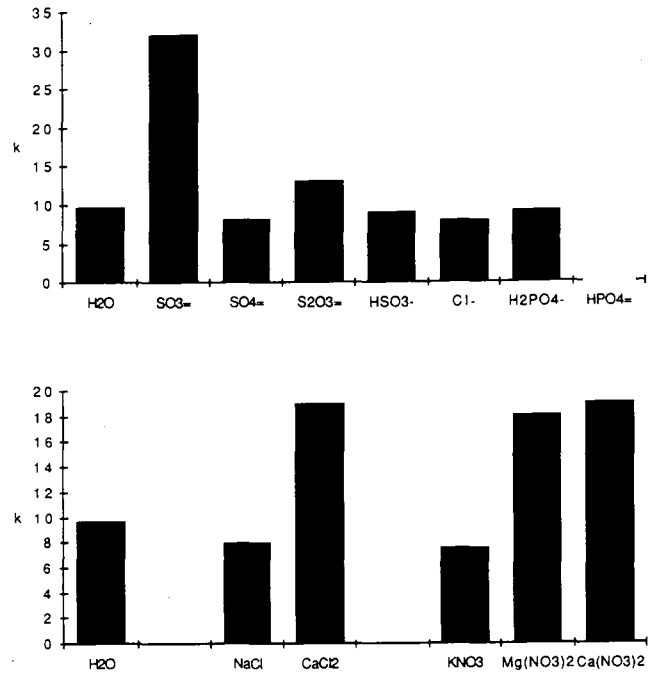


Figure. Effect of cations (upper) and anions (lower) on disulfate ion hydrolysis. (XBL 8811-3937)

The Chemistry of Bisulfite Ion in Aqueous Solution

D. Littlejohn, A. Li, and S.G. Chang

Bisulfite ion is the dominant form of SO_2 dissolved in aqueous solutions over a pH range of 2 to 7. Flue gas cleanup processes using aqueous solutions to remove SO_2 often have high concentrations of bisulfite ion. To properly treat these scrubbing solutions, the chemistry of bisulfite ion must be understood; however, it is fairly complicated. Bisulfite can exist in two isomeric forms and can form one- and possibly two- dimers. Using NMR, Horner and Connick[1] obtained a measure of the bisulfite isomerization equilibrium constant. They assigned NMR peaks to the isomers indirectly.

We have used Raman spectroscopy to observe the effect of temperature on low-concentration solutions of bisulfite ion. Spectra of solutions with pHs of 2.1, 4.2, and 6.6 were obtained at three temperatures: 278K, 298K,

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburgh Energy Technology Center, Pittsburgh, PA.

and 333K. The solutions had a concentration of 0.1M in total S(IV). From the temperature dependence of the peaks in the spectra, we were able to assign two previously unassigned Raman peaks. The 1023 cm^{-1} Raman band is from the $HOSO_2^-$ bisulfite isomer; the 1052 cm^{-1} band is from the HSO_3^- isomer.

The relative intensities of the bands were used to determine the equilibrium constant for the isomers. Because the strength of the Raman bands cannot be easily predicted, the 298K equilibrium constant value of Horner and Connick[1] was used to determine the intensity ratio of the 1023 cm^{-1} and 1052 cm^{-1} bands. With this information, we calculated the equilibrium constant as a function of temperature (Figure). No significant difference was observed between the three pH conditions. From the sum of the results, we obtain an expression for the equilibrium constant:

$$\ln K = (-\ 1.91 \pm 0.23) + (1032 \pm 70)/T$$

where $K = (HOSO_2^-)\ /\ (HSO_3^-)$. From this expression, values of $H = -\ 2.1 \pm 0.2$ kcal mol^{-1} and $S = -\ 4 \pm 0.5$ cal K^{-1} mol^{-1} are derived. Much more work must to be done on the chemistry of this system, including that associated with the dimer or dimers.

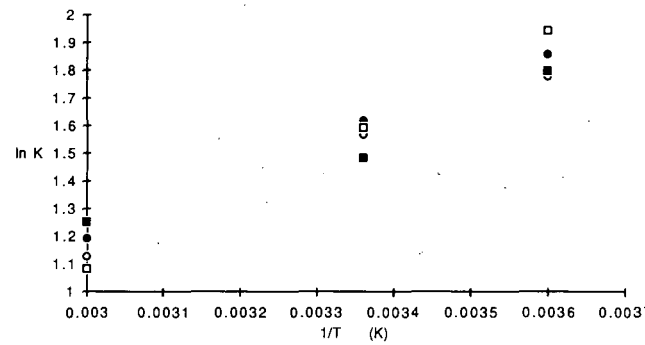


Figure. Plot of the log of $(HOSO_2^-)/(HSO_3^-)$ vs 1/T. Key: solid circle - pH 2.1, open circle - pH 4.2, solid square - pH 6.6, open square - values of Horner and Connick. (XBL 8811-3938)

REFERENCES

1. Horner DA, Connick RE. Equilibrium Quotient for the Isomerization of bisulfite ion from HSO_3^- to SO_3H^-. *Inorg Chem* 1986; 25:2414.

Controlled Combustion*

D.W. Faris, K. Hom, J.A. Maxson, A.K. Oppenheim, and H.E. Stewart

The major purpose of this study is to provide a scientific basis for developing controlled-combustion engines. Pragmatically, such engines have the prospect of minimizing the formation of pollutants, optimizing the tolerance to a wide assortment of fuels, and maximizing fuel economy. In order to attain such a goal, combustion chambers-considered so far as just sources of motive power-have to be converted into fully controllable chemical reactors. In principle, this involves a fundamental modification of the process of combustion in that, instead of having to rely on the Flame Traversing the Charge (FTC) system used universally today, combustion is carried out within regions of well-stirred reaction zones. This mode of combustion can be accomplished by a Pulsed Jet Plume (PJP), a turbulent plume formed by a pulsed jet generated by combustion in a cavity of an igniter plug of C type described previously.† Our studies became focused on exploring the prominent features of jet ignition and the dynamic effects of the exothermic process of combustion taking place within a predesignated elementary region of the reactor (the head space in an engine).

Further studies using our numerical modeling techniques and evaluation of fluid mechanics of flames propagating in enclosures[1–3] presented a basis for identifying the essential aspects of a controlled-combustion engine.[4] We also completed experimental tests of pulsed plasma jet igniters[5] and the computational investigations of the dynamic effects of exothermic combustion centers.[6]

Using our molecular beam mass spectrometer, we succeeded in measuring 1) species concentration histories in the plume of a pulsed plasma jet igniter during ignition and 2) subsequent combustion of methane/oxygen, nitrogen and methane/oxygen/argon mixtures. Equivalence ratios of 1.0, 0.6, and 0.4 were used in the igniter cavity and in the main combustion chamber to provide both combusting and non-combusting cases. Species measurements indicate that combustion initiated by plasma jets can be divided into three phases. The hot initial stage is dominated by high-temperature species formed in the plasma cavity and in the turbulent plume, entrainment continues in a second region, with generation of products in the plume but not in the bulk gas mixture. High radical concentrations characterize the first stage; N atoms peak at a mole fraction of 0.004, and OH reaches a value of 0.007 in the stoichiometric case. The second stage involves the reactions of intermediate products such H_2, NO, and CO along with the production of final, stable products. In the final stage, CO_2 and H_2O concentrations rise to levels expected from complete combustion of the reactants. These measurements are used to explain how pulsed plasma jets enhance ignition in lean mixtures.

We computed the dynamic effects of a local exothermic center for a number of representative gaseous fuel/air mixtures in cases where reliable chemical kinetic models are available. Fuels under consideration included hydrogen, methane, acetylene, ethylene, and ethane. This study was based on the premise that exothermic centers arise from inhomogeneities in the bulk mixture and ignite earlier than the surrounding mixture. The model of an exothermic center considers thus a small, homogeneous mass of reacting mixture surrounded by an essentially inert mixture. In the analysis, the energy and species equations for the reacting mixture are combined with the gas dynamic constraints for expansion of the exothermic kernel in the center. Induction time, excitation time (rise time of the exothermic power pulse), and exothermic energy and power of the centers are then evaluated. An important dynamic effect of the center is the compression wave it produces in the surrounding mixture. Computations show that compression ratios of 1.2 to 1.8 are achieved at elevated initial pressures in the exothermic centers we studied.

With this as a background, we turned our attention to the physics and chemistry of combustion in PJP's. Preliminary experiments were run in a constant-volume, cylindrical vessel, providing an unobstructed optical insight along the axis for schlieren photography. The progress of the exothermic process was monitored by pressure transducer records. The results demonstrated the superiority of this mode of combustion as compared with the FTC system tested under identical operating conditions and revealed the ability of a PJP to entrain (inhale) the surrounding mixture into its midst for chemical processing inside the region of space it occupies, being spread across the surroundings by a propagating (self-advancing) flame front. Further exploration of the characteristic features of combustion by PJP's have thus become the principal goal of our project.

To study the physical and chemical processes taking place in an exothermic PJP, experimental investigations will use a constant-volume vessel used for preliminary experiments and a shock tube to test the operating features of PJP's under high initial pressures and temperatures (as well as turbulence level) and resembling those of internal combustion engines.

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Engineering and Geosciences Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the U.S. Army Research Office under Contract No. DAAL03-87-K-0123.

†*Applied Science Division FY87 Annual Report*, p. 2-17 (Fig. 2), March 1988. (LBL-24212)

Associated with this, we will conduct an analytical effort to explore the mechanism of the flow field generated by a PJP, based on numerical modeling techniques we are currently adopting for this purpose.

REFERENCES

1. Rotman DA, Oppenheim AK. Aerothermodynamic properties of stretched flames in enclosures. *In: Twenty-First Symposium (International) on Combustion.* The Combustion Institute, 1986; 1303-1312.
2. Giovannini A, Oppenheim AK. Analyse de different types d'ecoulements internes par la methode des vortex aleatoires. *J Theoret App Mech,* 1987; *6*: 771-787.
3. Chau EL, Rotman DA, Schipperijn FW, Oppenheim AK, Sawyer RF, Iiyama A, Xia, LQ. Experimental and Numerical Modeling Study of Engine Combustion. SAE Paper 872103, 1987.
4. Oppenheim AK. Quest for Controlled Combustion Engines. SAE Paper 880572, 1988.
5. Lucas D, Cavolowsky JA, Breber PR, Oppenheim AK. Pulsed Plasma Jet Igniters: Species Measurements in Methane Combustion. Presentation at the 22nd International Symposium on Combustion, University of Washington, Seattle, WA, August 1988.
6. Lutz AE, Kee RJ, Miller, JA, Dwyer HA, Oppenheim AK. Dynamic Effects of Autoignition Centers for Hydrogen and $C_{1,2}$-Hydrocarbon Fuel. Presentation at the 22nd International Symposium on Combustion, University of Washington, Seattle, WA, August 1988.

Combustion Chemistry*

N.J. Brown and R.J. Martin

Chemical reactivity, energy transfer, transport processes, and fluid mechanics govern combustion processes. Our research is primarily concerned with understanding the first two of these so that better control over combustion can ultimately be achieved. Advances of theories of reactivity have important impacts on our understanding of the chemistry affecting the emissions of pollutant species, rates of heat release during combustion, and the growth rates of undesirable combustion phenomena.

Research continued on the use of functional sensitivity analysis[1] to measure the response of dynamical observables to arbitrary variations of the potential energy surface at given points in configuration space. This research is being conducted in collaboration with Herschel Rabitz and Richard Judson of Princeton University. Particular attention was given to representing the complete sensitivity functions for the two dimensional/two molecule/rigid rotator problem. In Figure 1, radial slices of these are shown for the HD molecule. Each panel shows the function for a fixed value of R, the separation between the center-of-mass for each molecule given in bohr. The abscissa is the polar angle of molecule 1 (H_2), while the ordinate is the angular coordinate for molecule 2 (HD). Solid contours indicate positive values; dotted contours indicate negative values. These contours provide direct evidence of molecule/molecule behavior.

Studies of rotational relaxation in the HD + HD system were completed, and energy transfer rates from more initial states were determined. Agreement between

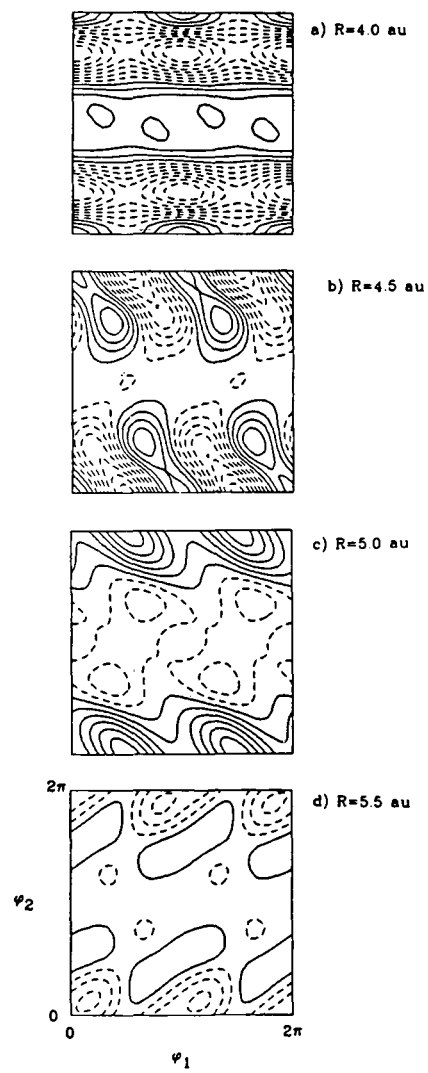


Figure 1. Radial slices of the full log-normalized sensitivity function for the change in rotational energy in HD. The ordinate and abscissa are given in polar angles for fixed values of the radial coordinate. (XBL 891-92)

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

theoretical and experimental rotational energy transfer rates was within an order of magnitude and was considerably better for transitions to neighboring states.

We performed a complete Monte Carlo calculation of the H_2 + OH rate coefficient for the temperature range 750 to 4000 K, and agreement with experimentally determined and transition state values was very satisfactory. Energy rejection techniques were used in this calculation, and these corrected for zero-point problems encountered in conventional quasi-classical approaches.

A review paper is being written on rate coefficient calculations for combustion modeling studies. Major topics in the review are potential energy surfaces, various forms of transition state theory, quasi-classical dynamics, and sensitivity analysis.

Research also continued[2] on the modeling of N_2O combustion chemistry; these calculations were performed in concert with sensitivity calculations. We are modeling premixed laminar flames where N_2O is formed and destroyed, and we have achieved excellent agreement between calculations and experiments.

We plan to pursue research on the functional sensitivity analysis as a tool for probing the mechanisms of molecular collisions. In addition, we expect to complete our review paper on rate coefficient calculations for combustion modeling studies. Modeling of our laminar flame experiments and flash-ignited combustion experiment will also be completed.

REFERENCES

1. Judson RS, Rabitz H, Brown NJ. A classical functional sensitivity analysis of coplanar inelastic scattering for $H_2 + H_2$ and its isotopic analogs. (*J Phys Chem*, in press, 1988)
2. Martin RJ, Brown NJ. The importance of thermodynamics to the modeling of nitrogen combustion chemistry. (*Combustion and Flame*, in press, 1988)

Combustion Fluid Mechanics*

R.K. Cheng, I.G. Shepherd, and L. Talbot

Turbulent combustion is the dominant mode of operation in most engines and burners because fluid mechanical turbulence enhances the burning rate. The coupling between turbulence and combustion chemistry is very complex, and the interactions involve significant temperature, velocity and pressure fluctuations in both space and time. Fluctuations affect reaction rate as well as concentrations in the combustion exhaust. Moreover, because the range of chemical and fluctuation time scales span many orders of magnitude, experimental studies and the development of turbulent combustion theory present major challenges to combustion scientists today.

One of the most viable means of gaining a better physical understanding of the controlling turbulence-combustion interaction processes is by investigating the combustion flowfields in laboratory scale burners. These experiments are designed so that the fluid mechanical time scales are large compared to the chemical time scales so that theoretical treatment of the combustion chemistry can be simplified. By use of laser diagnostic techniques which measure scalar and velocity fluctuations and other statistical cross-correlations, data are obtained for comparing and evaluating current theoretical models and for determining the effects of turbulence intensity on burning rates.

For premixed turbulent combustion studies where the fuel and the oxidizer are thoroughly mixed prior to combustion, we use three laboratory burners of different geometries: rod-stabilized "v" flames, large conical Bunsen type tube-stabilized flames, and planar flames stabilized in the stagnation flow. The burners are designed to provide the best possible data for comparison with current one-dimensional (1-D) or two-dimensional (2-D) theoretical models. One of our significant recent achievements is the development of an experimental procedure to trace the flow path through the flame zone. This procedure is based on automatic feedback control of a two-component laser Doppler anemometry (LDA) system which measures in-situ flow velocities. Examples of flowpaths determined within a methane/air v-flame are shown in Fig. 1. The flowpaths are clearly not aligned with the principal axes of the burner; therefore, previous measurements made along fixed vertical or horizontal axes may have led to erroneous conclusions. The physical significance of the flowpaths is also confirmed by the development of a novel method for determining overall burning rate, based on reaction-rate data obtained along these paths.

The statistics on velocity along the flowpaths also show the influence of burner geometry. This is due to flow acceleration induced by combustion heat release which modifies the characteristic pressure field of burners with different geometric contraints. Consequently, the turbulence intensity in the burned region depends on whether the pressure increases (as in the stagnation flow region) or decreases (as in the v-flames) downstream from the flame. Modeling of the evolution of the turbulence intensity within the flame zone requires empirical data. Because reliable diagnostic methods for measuring pressure fluctuations are not available, the velocity data remain the only means of inferring changes in the pressure field. We plan to continue our analysis of the velocity data along the flow paths. In particular, the magnitudes of the flow acceleration and changes in turbulence intensities will be compared for various flames with different turbulence and fuel/air ratios.

Another aspect of the flame-flow interaction which has not been explored in detail is the effect of the flame on the non-reacting region upstream of the reaction zone.

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

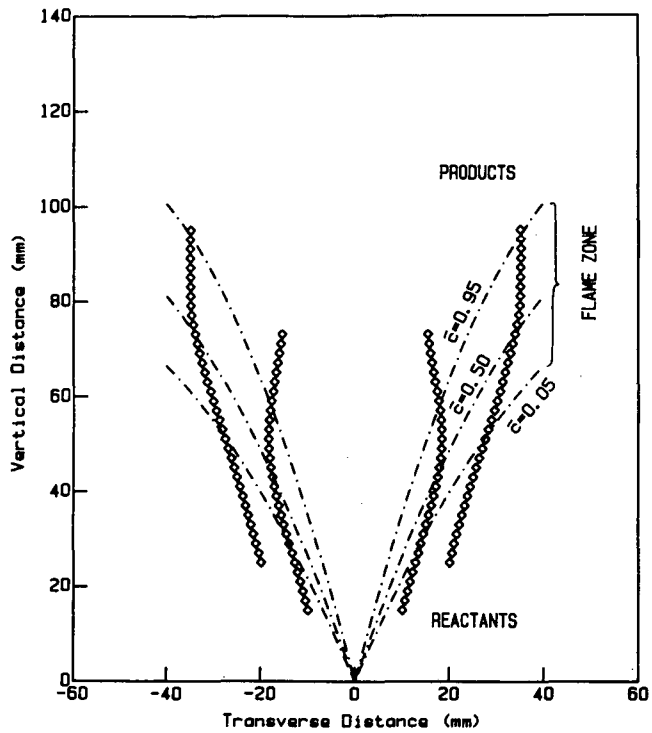


Figure Example of flowpaths through a methane/air v-flame as determined by automatic feed-back control of a 2 component Laser Doppler anemometry system. flow path positions. (XBL 8811-3853)

The velocity time scales deduced by spectral analysis show some changes. Comparison of the velocity time scales with the time scales of the temperature fluctuations within the reaction zone have provided some evidence that the two scales are related. Because the time scales of the temperature fluctuations are associated with reaction rate, such comparison will be useful for quantifying the relationship between turbulence intensity and burning rate. As most current models do not consider the effects of combustion in the upstream region, our investigation is expected to show whether or not these effects warrant theoretical treatment.

In FY88, we initiated two experiments for studying turbulent non-premixed (diffusion) flames. In non-premixed flames, mixing of the fuel and the oxidizer occur simultaneously with combustion. The flowfields are more complex than those of the premixed flames. The two experiments both use a fuel jet issuing into co-flow or opposed flow of air. The flow and mixture conditions are designed so that the turbulence time scales are large compared with the chemical times. Using various flow visualization techniques, we have thus far obtained preliminary data on the shape of the reaction zone. Measurement of the velocity statistics are well underway and will be continued.

In addition to our experimental efforts, progress has also been made in our numerical study of premixed turbulent flames using the vortex dynamic technique. The numerical work complements the experimental studies. We have explored means of improving the algorithm for describing the flame movements. The flame movement within the reaction zone consists of two components. The first is associated with the transport of the flame by the mean flow; the second is caused by flame propagation. Because flame propagation represents the fuel consumption rate, it is directly related to the turbulent burning rate. Previous algorithms assume that the flame propagates everywhere at a constant burning speed. This technique cannot consider the effects of flame curvature or the effects of flame cusps. A new flame movement algorithm developed by Prof. J. Sethian for vortex dynamic simulations of premixed turbulent flames is capable of overcoming these limitations, and this algorithm is being incorporated into our numerical program for the v-flames. The evolution of the shape of the flame interface predicted by this model will be compared with those obtained experimentally by tomography. Also deduced from the numerical results are the conditioned velocity statistics, which can be compared with previously obtained experimental data.

Smoke Emission Measurements from Medium Scale Experiments*

R.B. Williamson, R. Dod, C.M. Fleischmann, N.J. Brown, and T. Novakov

The concept of a "nuclear winter" has been postulated with a number of assumptions regarding the smoke produced by post-nuclear exchange fires. Knowledge of the quantity and character of the smoke emitted by those fires is crucial for predicting their climatic impact.

To help quantify the smoke which might be generated after use of nuclear weapons - and which may cause a "nuclear winter" - we conducted a series of medium-scale fire experiments using representative urban fuels such as wood, asphalt roofing, and liquid petroleum.

More than 20 medium-scale experiments were conducted in this research program. During each experiment, the mass smoke was determined by sampling the aerosol particulates in the exhaust duct which captured the effluent from the burning material, and the rate of heat release (RHR) was measured by oxygen depletion calorimetry (ODC). In addition, the characteristics of the smoke, and particularly its graphitic ("black") carbon content, were analyzed. Another important, unique aspect of this research is that some experiments were conducted with limited ventilation by burning materials in a compartment having only a window to admit air inside.

*This work was supported by the Defense Nuclear Agency through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The smoke emission factors measured for burning wood under well-ventilated conditions ranged from 0.1% to 0.3%, but under limited conditions this increased an order of magnitude, i.e., to between 1% and 3%.

For No. 2 fuel oil, the well-ventilated smoke emission factor ranged from 8% to 10%, but when the oil was burned in the compartment, the emission factor dropped to 5%. This experiment was not "ventilation limited"; approximately twice as much oxygen was present than would have been necessary for burning all the fuel volatilized per unit time. This decrease in emission factor for the oil burned in the compartment is probably attributable to the higher temperature resulting from radiative feedback in the compartment (as compared with the open pan fire) and to more complete combustion resulting in substantial soot burnout.

The smoke emission factors measured for asphalt under well-ventilated conditions were approximately 12%. Asphalt was not burned in the compartment.

In the context of a "nuclear winter," the implications of these measurements are centered around four concepts. First, ventilation has a substantial effect on smoke production from burning wood and oil; the emission factors for wood measured under limited ventilation conditions were more than an order of magnitude higher than those measured under well-ventilated conditions. More importantly, the smoke in the compartment fire was thick and black, similar in appearance to the smoke produced by burning plastic or oil. Wood is one of the major building and furnishing materials used in the United States, and we may reasonably assume that large quantities of wood would burn under both limited and unlimited ventilation conditions in the post-nuclear environment.

Second, the well-ventilated medium-scale wood experiments produced several orders of magnitude more black carbon than did previously reported bench-scale experiments. The black carbon particles absorb sunlight and produce the "nuclear winter" effects.

Third, the smoke emission factors for asphalt roofing shingles (a total of more than 12% with 90% being black carbon) could have a significant impact on urban smoke production in the post-nuclear environment.

Fourth, our experimental results to date show an important trend: the smoke emission factors for oil decrease as fire size or intensity is increased. The smoke emission factors were more than 10% for the single-pan experiments but decreased when the fire was doubled or placed in the compartment.

For FY 89, we plan to continue the medium-scale experiments with increasing rates of heat release under various ventilation conditions in order to evaluate the effects of scaling. In particular, we will emphasize the study of scaling between our experiments and will explore ways of correlating our findings with those of other investigators.

Photochemical Conversion of Solar Energy by Microbial Systems*

L. Packer, R.J. Mehlhorn, I.V. Fry, J.J. Maguire, S. Spath, G. Khomutov†, W. Nitchmann, E. Hrabeta-Robinson, M. Huflejt, J. Hrabeta, C. Reveron‡, J. Park, and K. Kondo

The Membrane Bioenergetics Group is investigating biological energy conversion mechanisms with reference to the roles played by membrane compartmentation, membrane structural components, and ion transport systems. Structure and function analyses are being integrated to present a complete picture of biological energy utilization. The use of salt (stress) is employed as a probe of bioenergetics in an obligate halophile (*Halobacterium halobium*) and in a fresh-water, halotolerant cyanobacterium (*Synechococcus* 6311).

H. Halobium

Intracellular pH was determined in cells loaded with the membrane-permeable precursor of the pH-sensitive fluorescent dye 2′, 7′-bis-(carboxyethyl)-5(6)-carboxyfluoresceinacetoxymethyl ester. The dye contains two carboxyl groups which are esterified with acetoxymethyl groups to yield an uncharged, membrane-permeable molecule. The permeable precursor is cleaved by cell esterases and the charged pH-sensitive dye remains trapped inside. This method proved to be a reliable indicator of internal pH and is currently being adapted to study the dynamic changes of cytosolic pH in response to changes in metabolism and environmental conditions in other bacteria.

Cyanobacteria

Magnetic resonance spectroscopy (electron paramagnetic and nuclear magnetic resonance) and gas chromatography have been used to determine the physical characteristics of the subcellular membrane systems with regard to viscosity, order parameter, and chemical composition. Major changes in viscosity and order parameter were observed in the cytoplasmic membranes but not in the thylakoid membranes under stress conditions. The lipid fraction exhibited modification in both membrane systems (an increase in the 18:1 fatty acid side chains). The data are consistent with an increase in the protein content of the cytoplasmic membrane. This finding is corroborated by increases in the number and size distribution of particles in the cytoplasmic membrane observed by freeze-fracture electron microscopy. We have developed several novel ESR and fluorescent methods that measure pH gradients inside cyanobacteria across both the cell and the thylakoid membranes. We have determined the effects of salt stress on intracellular pH and are developing a more detailed understanding of the ion channels in the cytoplasmic membrane. Our studies reveal that a major bioenergetic response which allowed cells to tolerate high salinity was a development of higher permeability to NaCl and increased respiration. Furthermore, from the response of internal volumes to various cations, the discovery of at least two different transport systems for Na^+ and NH_4^+ in control and salt-stressed cells can be deduced. One cation transport system is sensitive to amiloride, whereas the other is sensitive to L-methionine-D, L-sulfoximine. We have also developed an ESR method for measuring the concentration of oxygen inside living cells under conditions of active photosynthesis and respiration, and we have recently determined the highest concentration of oxygen observed so far in biological systems.

*This research was supported by the Office of Basic Energy Sciences of the U.S. Department of Energy under contracts DE-AC03-76SF00098 and DE-FG03-87ER13736 and NASA Interagency agreement A-14563c.

†A recipient of an IREX fellowship, under the US/Soviet exchange program.

‡LBL/JSU/AGMEF summer faculty program.

REFERENCES

1. Belkin S, Mehlhorn RJ, Hideg K, Hankovsky O, Packer L. Reduction and destruction rates of nitroxides. *Arch Biochem Biophys* 1987; *256*: 232-243.
2. Belkin S, Mehlhorn RJ, Packer, L. Determination of dissolved oxygen in photosynthetic systems by nitroxide spin-probe broadening. *Arch Biochem Biophys* 1987; *252*: 487-495.
3. Belkin S, Packer, L. Determination of dissolved oxygen in photosynthetic systems and protective strategies against its toxic effects in cyanobacteria. *In: Proceedings of the 2nd International Symposium held at Madurai*, on 11-14 December 1985. New Delhi: Today and Tomorrow's Printers and Publishers, 1987; 27-37.
4. Huflejt ME, Negulescu PA, Machen TE, Packer L. Na^+ and light-dependent regulation of cytoplasmic pH in cyanobacterium: *Synechococcus* 6311. *Biophys J* 1988; *53*: 616a.
5. Khomutov G, Packer L. Ion-binding properties of nonhomogenous biological membrane structure. (Submitted for publication, 1988)
6. Lefort-Tran M, Pouphile M, Spath S, Packer L. Cytoplasmic membrane changes during adaptation of the fresh water cyanobacterium *Synechococcus* 6311 to salinity. *Plant Phys J* 1988; *87*: 767-775.
7. McLaggen D, Belkin S, Packer L, Matin A. Electron spin resonance measurements of the effect of iono-

phores on the transmembrane pH gradient of an acidophillic bacterium. (Submitted for publication, 1988)
8. Nitschmann WH, Packer L. EPR studies on proton gradients and Na^+-NH_4^+ exchange during salt adaptation of Synechococcus 6311. *In: Proceedings of the 5th European Bioenergetics Conference, Aberystwyth*, 20-26 July 1988. (in press, 1988)
9. Packer L. The bioenergetics of stress responses in cyanobacteria. *In: Proceedings of Indo-US Workshop on Applications of Molecular Biology in Bioenergetics of Photosynthesis*, Delhi, India, 4-8 January 1988. (in press, 1988)
10. Packer L. Stress responses in cyanobacteria. *In: Receptors, Membrane Transport & Signal Transduction* [NATO ASI Series *Cell Biology*]. (in press, 1988)
11. Packer L, Hrabeta E, Robinson AE, Abdulaev NG, Kiselev AV, Taneva SG, Toth-Boconadi R, Keszthelyi L. Effect of cross linkers on the bacteriorhodopsin photocycle. *Biochem Biophys Res Comm* 1987; *145*: 1164-1170.
12. Packer L, Hrabeta-Robinson E, Stefka-Hristova G, Toth-Boconadi R, Keszthelyi L. Proton translocation by chemically modified bacteriorhodopsin. *Biochem In* 1987; *14*: 977-985.
13. Packer L, Spath S, Martin JB, Roby C, Blingy R. ^{23}Na and ^{31}P NMR studies of salt (NaCl) stressed fresh water cyanobacteria. *In: Proceedings of the 4th International Conference on Water and Ions in Biological Systems, Bucharest, Romania, 24-28 May 1987*, 1988; 335-346.
14. Tsujimoto K, Semadeni M, Huflejt M, Packer L. Intracellular pH of halobacteria can be determined by the fluorescent dye 2',7'-bis(carboxyethyl)-5(6) carboxyfluorescein. *Biochem Biophys Res Comm* 1988; *88*: 123-129.

Detection and Prevention of Biological Free Radical Damage*

R.J. Mehlhorn, J.J. Maguire, K. Moore, B. Stone, J. O'Neil-Gonzalez, L. Packer and H. Rapoport

The study of oxidative free radical damage may prove to be the next major frontier of biological research, with profound implications for human welfare, including disease prevention and lifespan extension. The Membrane Bioenergetics Group has pioneered methods to detect free radicals and has applied these to both animal and plant systems.

*This work was supported by NIH (AG-04818) and LBL Director's funds for innovative research through the U.S. Department of Energy under contract DE-ACO3-76SF00098 and by the National Foundation for Cancer Research.

This project develops and applies ultrasensitive and non-destructive assays of oxidant stress in animals seeks to elucidate mechanisms of antioxidant action, including how vitamins C and E protect animals against free radicals. Our principal experimental approach is to use electron spin resonance (ESR), which detects magnetic moments associated with the unpaired electrons present in all free radicals. This basic approach is rendered highly sensitive by means of "free radical traps" that accumulate products of free radical reactions. We have developed such traps for detecting oxygen-, sulfur-, and carbon-centered free radicals, free transition metal ions, and non-radical oxidants that can be activated to form free radicals. In addition, we are developing a new chemical method whose basis is a radiolabeled chemical that can be injected into an animal, whereupon its reaction with hydroxyl and other strongly reactive oxyradicals causes the chemical to decompose into several fragments including a small, radiolabeled hydrocarbon fragment that will be volatilized in the lung and can be detected in expired breath.

Synthetic Work

We have implemented successful synthetic procedure for preparing the chemical free radical trap, alpha-keto-gamma-methylbutyric acid (KMBA), labeled so that ethylene derived from it contains a hydrogen isotope. The yields in this process are good, the compounds are stable and easily purified, and the hydrogen isotope is introduced via sodium borohydride. Since sodium borohydride of high specific activity is now available as a result of developments in the National Tritium Labeling Facility, we project liberated ethylene of specific activity ~25Ci/mmole from the labeled KMBA. We are studying release of ethylene from unlabeled and labeled KMBA, incorporation of tritium into KMBA, and development of more efficient analyses for the released ethylene.

Preparation of an ESR Probe of Transition Metal Ions and Buffer Purification Procedure

Treatment of the "stable" free radical 4-hydroxy-2,2,6,6-tetramethyl piperidine-N-oxyl (Tempol) with excess ascorbic acid reduced the nitroxide to its diamagnetic hydroxylamine, 4-hydroxy-2,2,6,6-tetramethyl piperidine-N-ol (designated as TOLH). TOLH undergoes only one-electron oxidation, making it suitable for free radical and transition metal ion detection. Initial experiments with TOLH revealed considerable variability of oxidation rates among different buffers, due to contamination with transition metal ions. An effective purification procedure was found to be treatment of the buffers with insoluble sodium phosphate glass, whose high negative charge density attracted the multivalent cations from the bulk aqueous phase, allowing them to be precipitated with the phosphate glass. Treatment of TOLH with cupric ions (cupric sulfate) catalyzed rapid oxidation to the nitroxide. Under aerobic conditions, this oxidation proceeded until all TOLH had become oxidized. Chelation of the copper with EDTA brought this oxidation to a virtually halt. Aqueous

ferric ion oxidized TOLH relatively slowly, but this rate was markedly accelerated by EDTA. Treatment with EDTA is thus a simple method for discriminating between copper and iron.

Detection of Thiyl Radicals with a Pyrroline Nitroxide

A Proxo nitroxide resistant to one-electron reduction by mild reducing agents like ascorbate was used to detect thiyl radicals. Glutathione was oxidized to thiyl radicals both chemically and enzymatically. The ESR signal of the nitroxide disappeared in buffered glutathione solutions aerobically but was quite stable under anaerobic conditions. Addition of traces of hydrogen peroxide to anaerobic glutathione caused rapid decreases in the nitroxide ESR signal, with more than three equivalents of nitroxide lost relative to the concentration of added peroxide. This non-enzymic reaction of nitroxides with glutathione was due to transition metal ions, since treatment with chelating agents inhibited the activity. A plausible mechanism of thiol activation is interaction of ferric ion with hydrogen peroxide to form the ferryl species, which abstracts a hydrogen atom from glutathione to form the glutathionyl radical. Glutathionyl also reacts with glutathione to form a species that reduces nitroxides to hydroxylamines. With horseradish peroxidase, phenol and hydrogen peroxide Proxo was both reduced and destroyed. Participation of thiyl radicals was confirmed by demonstrating that Proxo destruction was competitively inhibited by the spin trap DMPO, whose glutathionyl adduct was observed to increase to the same extent that Proxo destruction decreased.

The Production of Free Radicals by Thyroid Peroxidase

Peroxidase enzymes are well known to generate powerful oxidants in vitro. ESR measurements of TOLH oxidation have shown that can be used to accurately measure hydrogen peroxide, peroxidase activity, and phenol activity in tissue. We have applied TOLH to thyroid preparations from a variety of animals and demonstrated free radical production by peroxidase enzymes with an exogenous source of hydrogen peroxide and several phenols. We have thus established that enzymes present in animals can generate potent free radicals, provided that sufficient hydrogen peroxide and phenolic equivalents are present.

Bilayer Permeability of Liposomes to Methyl Radicals

A flavin-based photochemical system for generating methyl radicals outside asolectin liposomes was used to demonstrate that these radicals readily cross bilayer membranes. The liposomes were prepared such that an impermeable nitroxide was trapped inside them. Photochemical generation of methyl radicals outside the liposomes destroyed both internal and external populations of the nitroxide (as seen in the decay of their ESR signals), demonstrating that lipid bilayers are not effective barriers to the movement of alkyl radicals. This is important for understanding free radical mutagenesis and carcinogenesis because it demonstrates that lipid peroxidation products from metabolically active membranes like mitochondria can migrate across the nuclear membrane to interact with DNA.

Studies of One-Electron Tocopherol Oxidation and Reduction

The tocopheroxyl radical was observed by ESR in liposomes containing physiologic concentrations of alpha-tocopherol. The one-electron oxidation of tocopherol was catalyzed by horseradish peroxidase and the hydrophilic phenol arbutin with either direct addition of hydrogen peroxide or with a glucose oxidase system. In di-oleyl phosphatidyl choline liposomes, the tocopheroxyl radical could be observed for several hours with the glucose oxidase system and, after an initial decay period, a residual fraction of the alpha tocopherol was also stable. These results indicate that under appropriate conditions in biomembranes, the tocopheroxyl radical can be stable and that radical dimerization is not a facile pathway for its destruction. We also applied this enzymic oxidizing system to liver microsomes and submitochondrial membranes and showed that the tocopheroxyl radical could be produced in sufficient concentrations to be ESR-detectable in membranes isolated from rats that had been fed vitamin E-enriched diets. The radical in the subcellular membranes was also stable in the presence of the enzymic generating system but decayed rapidly when enzyme activity was arrested by removing oxygen.

Impacts and Multiple Iridium Anomalies*

F. Asaro, H.V. Michel, L.W. Alvarez‡, W. Alvarez†, and A. Montanari†

A geochemical study has been made of nearly 60 meters of limestone deposited during a period of 5 million years near the Cretaceous-Tertiary (K-T) boundary in the Bottaccione Gorge near Gubbio, Italy. Except in 2.6 meters of rock directly adjacent to the huge K-T iridium (Ir) spike, no Ir anomalies were observed, and the average Ir background was 12.6 x 10^{-12} gram of Ir per gram of rock (ppt). Close to the spike, however, are about a dozen Ir peaks ranging from 20 to 80 ppt above background.

In a study with H.R. Bowman, we observed that the Ir peaks in the Tertiary disappeared when ratios were taken to abundances of elements in clay, e.g., Fe, Si, and Al. The continuous and nearly exponential nature of the resulting curves suggests that the deposition of Ir was not episodic, and so the Ir is not due to volcanism or impacts of comet clusters. Washing of the continents following the K-T impact is a possible Ir source.

The Cretaceous Ir peaks, on the other hand, do not disappear when ratios are taken to the abundance of clay elements, and they may be due to diffusion.

Multiple Ir anomalies have been detected in Late Eocene deposits (impact-related) and (with Erle G. Kauffman) at the Cenomanian-Turonian boundary (probably mantle-related).

A single Ir peak in 11.7-million-year-old sediment has been observed (with Mark H. Anders) in one location (DSDP hole 588B) in a study of a continuous 53-meter section.

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division, of the U.S. Department of Energy under Contract No. DE-ACO3-76SF00098.

†Department of Geology & Geophysics, University of California, Berkeley, CA 94720

‡Emeritus Professor of Physics, University of California, Berkeley. Professor Alvarez died September 1, 1988.

A Study of the Relation Between Volcanism in the Weddell Sea about 65 Million Years Ago and the Cretaceous-Tertiary Bolide Impact*

H.V. Michel, F. Asaro, W. Alvarez†, and L.W. Alvarez‡

In a study of cores from ODP Hole 689B, no iridium (Ir) anomaly was found in sections 1 through 6 of core 25 or in core 26 from the top down to section 2, 3-12 cm. The background in clay-poor sediments averaged 11 parts-per-trillion (ppt) Ir, and a clay-enriched region had nearly the same average, 26 ± 12 ppt. If the Cretaceous-Tertiary (K-T) contact is in the region studied, then the K-T boundary was probably either not deposited or it was eroded away.

In a study of cores 15 and 16 of ODP Hole 690C, an iridium peak of 1566 ± 222 ppt was found in section 4 of core 15, 39-40 cm with a half width of 6.6 cm. Background abundances were ~15 ppt, and distinctly higher Ir abundances were observed from 119 cm below to 71 cm above the main peak. The Ir abundances were measured with the Iridium Coincidence Spectrometer (ICS) following neutron activation. The abundances of many other elements were measured by conventional techniques of gamma ray spectrometry after neutron irradiation. Iron abundance data and ratios of the abundances of Ir, Sc, Cs and Co to those of iron are shown (Figure).

The main Ir peak occurs where the fossil forms change from Cretaceous to Tertiary, and this peak has been shown to be due to an impact on the Earth of an asteroid or comet about 10 km in diameter. The Ir distribution below the main peak is attributed to bioturbation by organisms with burrows extending at least 0.4 meter.

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division, of the U.S. Department of Energy under Contract No. DE-ACO3-76SF00098.

†Department of Geology & Geophysics, University of California, Berkeley, CA 94720.

‡Emeritus, Professor of Physics, University of California, Berkeley. Professor Alvarez died September 1, 1988.

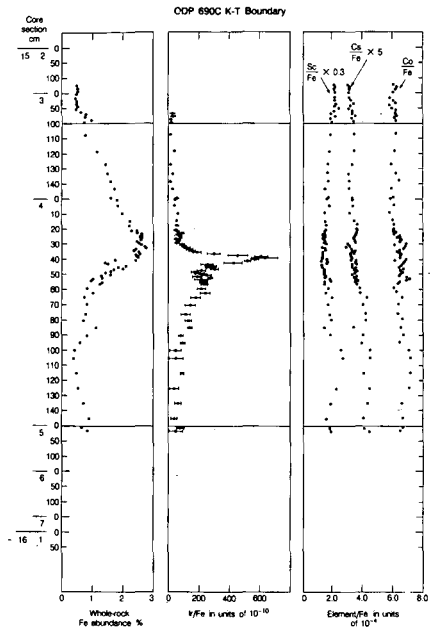


Figure. Ocean Drilling Program Leg 113 Hole 690C K-T Boundary. (XBL 889-8541)

The Ir distribution above the main peak may have the same cause, but other explanations may be significant.

In this work, we wished to determine whether volcanism in this region might have been triggered by the K-T impact. Clay, an alteration product of volcanic glass, is sometimes taken as an indication of volcanism.

The mainly $CaCO_3$ sediment of core 15 contains variable enrichments of clay, and the onset of the most intense deposit is found (within 2 cm) in the same position as the main Ir peak. The clay deposit, estimated to be about 50% of the sediment, extends upward ~19 cm and then slowly decreases to a background level of 10% over 1 meter. The degree of homogeneity of the clay deposit suggests it was not caused by episodic volcanism but may have been caused by a decreased $CaCO_3$ deposition rate possibly triggered by the K-T impact.

Sources of Quartzite in Ancient Egyptian Sculptures*

F.H. Stross, R.L. Hay[†], F. Asaro, H.R. Bowman, and H.V. Michel

Despite its great hardness and toughness, which makes it difficult to work, quartzite was used frequently in ancient Egypt in sculptures and architecture. Several quartzite deposits are known in Egypt, but the artifacts studied at the Lawrence Berkeley Laboratory appear to have derived from only two major deposits: Gebel el Ahmar (located near Cairo) and an area encompassing three contiguous quarries opposite and just north of Aswan. The LBL studies were made on the Colossi of Memnon in the Plain of Thebes and on a number of quartzite deposits known to have been (or which could have been) worked. The Gebel el Ahmar and Aswan quarry samples could be readily distinguished from other quarry samples by low abundances of calcium, manganese, and sodium.

The Gebel el Ahmar quarry is located about 680 km north and downstream from the Plain of Thebes, where the Colossi repose; the Aswan quarries are about 210-220 km south of Thebes. In our previous work, we found that the Colossi originally were made from rock taken from the Gebel el Ahmar quarry, whereas the blocks used by the Romans 1600 years later for large-scale reconstruction of the northern Colossus came from the Aswan deposit.

Knowing that the quartzite originally used for the Colossi came from the Cairo quarry, we are interested in discovering the sources of other artifacts of that era. In earlier work during the first field trip, a number of samples were collected from sculptures other than the Colossi. These and additional samples came from artifacts originally located at Thebes and its vicinity and also near Cairo; the samples include carvings from the reigns of kings of the New Kingdom (sixteenth to eleventh centuries B.C.).

The specimens under study were subjected to neutron activation analysis (NAA). Some of the specimens were

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

[†]Department of Geology, University of Illinois, Urbana, IL 61801.

also subjected to petrographic studies. Results of the NAA and petrographic studies, with the possible exception of samples with ambiguous or questionable provenience show that stela (or false door of Tutankhamen) in Thebes is the only object in the suite that appears to have used Aswan rather than Gebel el Ahmar quartzite. It would have been made little more than two decades after the death of Amenhotep III and would be the first quartzite carving shown to have used Aswan quartzite in pharaonic times. Later use is demonstrated by the unfinished obelisk of Seti I, still located in the Aswan quarries and which would have been carved about half a century after the reign of Tutankhamen.

REFERENCE

1. Stross FH, Hay RL, Asaro F, Bowman HR, and Michel, HV. Sources of the Quartzite of some Ancient Egyptian Sculptures. *Archaeometry* 1988; 30(Pt 1): 109-119.

Possible Worldwide Middle Miocene Iridium Anomaly and its Relation to Periodicity of Impacts and Extinctions*

F. Asaro, W. Alvarez[†], H.V. Michel, L.W. Alvarez[§], M.H. Anders[†], A. Montanari[†], and J.P. Kennett[‡]

In a study of one million years of Middle Miocene sediment deposition in ODP Hole 689B in the Weddell Sea near Antarctica, a single iridium (Ir) anomaly of (44 ± 10) x 10^{-12} gram Ir per gram rock (ppt) has been observed in core 6H, section 3, 50-60 cm, after background contributions associated with manganese precipitates and clay are subtracted. ODP Hole 689B is 10,000 km away from another site (DSDP Hole 588B in the Tasman Sea north of New Zealand), where a single Ir anomaly of 144 ± 7 ppt over a background of 11 ppt (core 25, section 2, 20-30 cm) was found in an earlier study of 3 million years of deposition. From chemical measurements the latter deposition was thought to be impact-related. Ir measurements were made with the Iridium Coincidence Spectrometer after neutron activation.

The age-versus-depth calibration curves given in the DSDP and ODP preliminary reports indicate the ages of the Ir anomalies are identical (11.7 million years), but the absolute and relative uncertainties in the curves are not known. Based on the newest age data, the age estimate is 10 million years.

Because the Ir was deposited at the two sites at about the same time (within our ability to measure) and the sites are one quarter of the way around the world from each other, the deposition seems likely to have been worldwide. The impact of a large asteroid or comet could produce the wide distribution, and the data support of impact relationship deduced for DSDP 588B from the chemical evidence. If the surface densities of Ir at the two sites represent the worldwide average, the diameter of a C1-type asteroid containing the necessary Ir would be 3 ± 1 km, large enough to cause worldwide darkness, and hence extinctions. This would be the third worldwide stratigraphic horizon of impact-related Ir-enriched rocks found, their ages being 65-66.7 (K-T boundary), 37-39.4 (Late Eocene), and 10-11.7 (Middle Miocene) million years. This spacing suggests a periodicity of 27-28 million years for the impact of large extraterrestrial bodies in agreement with those reported for extinctions and crater ages although both of the latter have been disputed.

Another stratigraphic horizon of Ir-enriched rocks has been observed in rocks about 91-92 million years old from North America, Italy, and Poland. Some of the rocks have a mantle signature, but the possibility of an impact on the ocean bottom cannot be ruled out as the source of the anomaly. An impact-related horizon has been observed in 2.3-million-year-old rocks distributed over 600 km. The minimum size of the bolide was reported as 0.5 km, which may be borderline for producing worldwide darkness. Anomalous Ir abundances have been observed at the Callovian-Oxfordian boundary in Spain and Poland. The origin of the Ir has not yet been well determined, and the chronological age is uncertain by many millions of years. Precambrian impact-related Ir deposits have been found in rocks about 3.5 billion years old in South Africa and possibly Australia; these rocks are too old to check the correlation with the observed periodicity.

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
[†]Department of Geology and Geophysics, University of California, Berkeley, CA 94720.
[‡]Department of Geological Sciences, University of California, Santa Barbara, CA 93106.
[§]Emeritus Professor of Physics, University of California, Berkeley. Professor Alvarez died September 1, 1988.

ENERGY ANALYSIS PROGRAM STAFF

Mark Levine, Program Leader‡
Ronald Ritschard, Deputy Program Leader‡
Michael Rothkopf, Deputy Program Leader‡

Hashem Akbari
Barbara Atkinson*
Barry Barnes
Sarita Bartlett
John Beldock
Didier Borderon*
Tom Borgers*
Betty Bratton
James Bull
John Busch
Stephen Byrne
Charles Campbell
Kathleen Carlson
Peter Chan
Mark Christensen
Deborah Connell
Paul Craig†
Philip Cunliffe
Marie DeBurge*
Yum Donggwan*
Susan Ellis
Joseph Eto
Anthony Fisher
Sunita Gandhi
Charles Goldman
Mark Goralka
Kathleen Greely
Steven Greenberg*
William Hanneman
Jeff Harris‡
Diane Hawk
Kristin Heinemeier*
Norbert Hirt*
Yu Joe Huang
Yizhu Huang*
Gilberto Jannuzzi*
Edward Kahn
Andrea Ketoff
Margaret Knight
Jonathan Koomey
Florentin Krause
Wilson Lai*
Feng Liu*
Christopher Marnay
Philip Martien*
Antonella Marucco*
Bartlett McGuire
Elizabeth McGuire
James McMahon
Alan Meier
Stephen Meyers
Evan Mills
Bruce Nordman
Richard Norgaard
Karen Olson
Samuel Oren
Park Chun Hun*
Soo-Hun Park*
Woo Park*
Mary Ann Piette
Giancarlo Pireddu*
Leo Rainer
John Randolph
Itzhak Ravid*
Paolo Ricci
Itzhak Ravid*
Henry Ruderman
Jayant Sathaye
Lee Schipper‡
Nancy Schorn
Renee Slonek
Steven Stoft
Haider Taha
Isaac Turiel
Dorothy Turner
Robert Twiss
Stephen Tyler
Edward Vine
Walter Westman
Deborah Wilson
David Wood
Winifred Wood

*Participating guest
†University of California at Davis
‡Group leader

ENERGY ANALYSIS PROGRAM*

INTRODUCTION

The Energy Analysis Program continues to be involved in wide range of topics relating to the energy system of the United States and numerous other countries. Our interest in energy use and conservation in buildings has remained high, with increasing attention being devoted to studies of commercial buildings. The appliance standards continues to be the leading energy policy analysis activity of the Program. A long-term commitment to characterizing and understanding measured data of energy use in buildings continues. Interest in electric utility issues, with particular emphasis on demand-side activities and programs, continues high. New interest in competition among electricity generation options for utilities complements the demand-side analyses.

The involvement in international energy studies has increased from previously high levels, with no waning in the commitment to the detailed analysis of factors affecting energy use by end-use. Building energy policy studies in the countries of the Association of South East Asian Nations continue to combine the Program skills in international studies, building energy analysis, and policy studies. An increased involvement in China has been of particular note during the past year.

The environmental initiatives of the previous year saw some important results, as analyses of effects of climate change on vegetation in California and habitat change and species extinction were completed. These efforts indicate success in the effort to significantly broaden the interests of the Program.

A new and potentially critical theme emerged and took hold in the energy and environmental communities during the past year: the potential for global warming. The Program has become involved in a variety of initiatives and analyses relating to this important topic. Data on energy demand growth in developing countries were analyzed in greater depth than previously in order to support the efforts of the Environmental Protection Agency (EPA) to understand measures to stabilize the atmosphere. Data on electricity use in developing countries were assembled to support longer-term efforts by the U.S. Department of Energy to assess the impact of electricity use in developing countries on global climate change. Studies of effects of increased temperature levels on selected vegetation types were initiated for the EPA. Numerous additional projects were designed to deal with key issues relating to global climate change, including a number of efforts with the Peoples Republic of China. Some or many of these are likely to be carried out over the next several years.

The year saw few major new problems in the energy economies of nations, with energy prices remaining relatively low and supplies in ample quantities. As a result, energy continued to play a small role in the national political scene. Nonetheless, the energy policy community continued to take note of the fact that low oil prices will not last forever, and possibly not even for another decade. There has been growing concern about an energy efficiency "plateau," resulting from low energy prices and reduced incentives to continue to improve the energy performance of economies. The advent of much more broad-based concerns about global warming has raised the recognition of the importance of long-term energy issues, even while the current situation appears manageable. It is in this broader context that new areas for energy analysis are likely to develop in the Program over the coming years.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems, Building Services, and Building Equipment Divisions, the Office of the Assistant Secretary for Environment, Safety, and Health, the Office of Policy, Planning and Analysis, of the U.S. Department of Energy; the U.S. Department of Housing and Urban Development under an Interagency Agreement (IAA-H-87-59); the Agency for International Development; the National Science Foundation under Interagency Agreement No. BSR-8717168; the NASA Earth Sciences Division (UPN-677-80-06-05); the Environmental Protection Agency under Interagency Agreement No. DW89933219-01-0; the Residential/Commercial Technology Analysis Division of the Gas Research Institute under GRI Contract No. 5085-800-1318; the Electric Power Research Institute; through the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

Utility Accounting in Public Housing

R. L. Ritschard and K. M. Greely

Public housing currently provides shelter and energy for over 3.4 million low-income tenants. Annual energy costs to the federal government for the public housing sector now exceed $1 billion. Preliminary studies indicate savings as high as 50% could be realized by improving the energy efficiency of the public housing building stock. These savings have not been realized, partly because local public housing agencies lack relevant energy-related information.

We have developed a utility accounting microcomputer program (based on Lotus 1-2-3® spreadsheets) that allows local housing agencies to track use electricity, gas, oil, other fuels, water, and sewer easily and accurately within individual housing projects. After a user enters monthly utility usage and costs into the program, it will adjust utility usage and costs to calendar months and convert consumption to common units (e.g., therms or cubic feet of gas and kWh of electricity to Btus of energy); weather-correct energy usage to that which would have occurred in a year having typical weather; compare each year's consumption and costs to previous years; and compare the consumption per unit-month to that in typical public housing apartments or privately-owned apartments having similar climate and building characteristics. The software helps produce executive summaries and other tables and graphs (see Figure) for tracking utility usage and costs across different years. The program also combines for analysis utility data for all projects within a public housing agency, calculates the allowable utility expense levels, and prepares two important annual reporting forms required by the U.S. Department of Housing and Urban Development (HUD). The output of the program can be used to verify proper rate payment, identify excessive energy use at given projects or buildings, and determine whether savings from previous energy retrofits have persisted over time. The software can also be used by local public housing agencies and by HUD to explore opportunities for reducing utility bills and to locate buildings and equipment requiring maintenance. We expect the program and documentation to be available by the end of 1988. These will be widely disseminated to local public housing agencies through the HUD User Network, which reaches more than 2600 U.S. housing agencies.

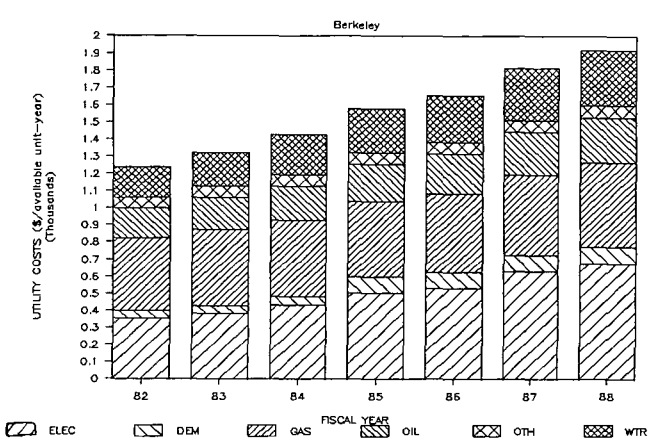


Figure. Sample energy computation produced by utility accounting program: annual utility costs per available unit. (XBL-891-159)

Energy Management Practices in Public Housing

E. Vine

To balance their budgets, U.S. public housing authorities (PHAs) must spend less energy. We have evaluated successful energy management practices conducted by U.S. public housing authorities. The study was undertaken to help other housing authorities learn how to manage their energy use. Housing authorities were selected primarily through interviews with U.S. Department of Housing and Urban Development (HUD) headquarters and regional offices; PHAs actively trying to manage their energy use were potential candidates for a mail survey.

An energy management survey was sent to 49 PHAs, yielding an 84% response rate. Topics addressed included energy actions, energy information, key energy actors, energy audits, program participation, financing and information sources, site description, energy management, maintenance, tenant involvement, type of metering, appliance purchasing criteria, energy use in 1980 and 1987, energy conservation measures installed, problems in managing energy, and problems in installing energy conservation measures.

We present below selected preliminary results from this study: all PHAs reported that they had saved energy since 1980; all PHAs had conducted energy audits; most PHAs (80%) had prepared an energy management accounting report; about 50% of the PHAs used in-house computers for tracking energy and cost data; about 40% of the PHAs had prepared a written energy plan for controlling energy costs, and 80% of these were currently using the plan; almost all PHAs had a preventative maintenance program; estimated average energy savings from retrofits was reported to be 21%; and the most effective energy conservation measures were insulation, window replacement, boiler replacement, and lighting conversions.

In FY 1989, we will continue analyzing these data, using multivariate statistical analysis to group these factors that determine successful energy management. We will also test several hypotheses concerning organizational change as it affects energy management.

Energy Requirements for Multifamily Buildings

R. L. Ritschard and Y. J. Huang

Over the past few years, multifamily buildings have been the most rapidly growing residential sector. As a result, multifamily housing has become an important sector of the energy economy.

LBL has contracted with the Gas Research Institute (GRI) to use the DOE-2.1C computer program to develop a comprehensive data base of hourly heating and cooling loads for prototypical multifamily buildings. This data base, covering 16 building types in 15 U.S. cities, reflects regional variations in climate, building construction and insulation practices, and represents the general population of multifamily buildings. Our major research goal is to provide GRI and its contractors with a reference set of building loads for use in planning and analyzing R&D programs in gas technology. The results also provide a general reference set of multifamily energy requirements for use by energy analysts. The full data base, which includes hourly heating and cooling loads (sensible and latent), domestic hot water loads, and electric consumption for each apartment unit and for the total building, will be available as part of this project.[1]

The Figure shows several important features representative of multifamily buildings. First, smaller buildings with 2-4 units usually have higher energy requirements per square foot than do multistoried buildings of five or more units. Second, energy use in older buildings is generally greater than that of newer ones. Third, in a southern climate like Atlanta, energy use for cooling may be equal to or greater than that for space heating. Finally, heating loads were more affected by improvements in thermal integrity (representative of newer buildings) than were cooling loads.

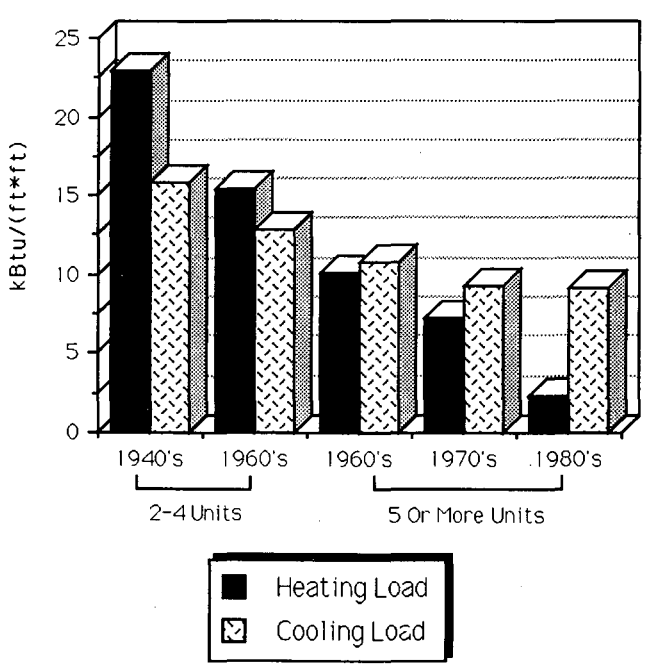


Figure. Estimated heating and cooling loads (per square foot) in typical multifamily buildings, Atlanta, GA. (XBL-8810-3732)

Due to the size of this data base, an interactive microcomputer program is being developed that will allow users to derive monthly loads, hourly profiles, or loads binned in different formats (e.g., by temperature and humidity ratio or by temperature and hour of day). In the next year, we will begin to use some of these data to assess different multifamily technologies. (See next article for a preliminary comparison of central vs. individual heating, ventilation, and air-conditioning (HVAC) and domestic hot water (DHW) systems in multifamily buildings.)

REFERENCE

1. Ritschard RL, Huang YJ. *Multifamily heating and cooling requirements: assumptions, methods, and summary results*, LBL-25727 draft report, 1988.

A Comparison of Central vs. Individual HVAC and DHW Systems in Multifamily Buildings

S.J. Byrne

Separate energy billing for apartments motivates energy-conscious occupants to control their energy use; such billing is facilitated by individual all-electric heating, ventilating, and air-conditioning (HVAC) systems and domestic hot water (DHW) systems. On the other hand, large, central systems are more efficient, require less maintenance, last longer, and allow more flexibility in choice of energy type. This project provides information on tradeoffs between individual and central HVAC and DHW systems in terms of energy performance and life-cycle costs in two climates, for different types of new multifamily buildings, and under varying operating conditions.

Using the DOE-2.1C computer program to model energy consumption in two typical apartment buildings—one in Chicago, the other in Atlanta—we analyzed two HVAC/DHW configurations per building; a central system consisting of a central chiller and gas-fired boiler which supply four-pipe fan coils (FPFC) and a gas-fired DHW system; and an individual system consisting of packaged terminal air-conditioners (PTAC) and electric water heaters in each apartment. To approximate energy-conserving operation, the individual PTAC system was modeled with and without a setback thermostat. We used each city's average prices for energy and equipment.

For both cities in our analysis, projected annual energy costs were lowest for the central HVAC/DHW system. This was especially true for Chicago because of its higher heating demand and higher price differential between electricity and natural gas. A life-cycle cost comparison of system types showed that in Chicago, multifamily buildings with more than seven apartments (in Atlanta, more than thirteen) should be designed with central HVAC and DHW systems.

Shown below is an example plot of life-cycle cost vs. number of apartments. The intersecting lines at "A" illustrate the point at which the system type should be changed to achieve the lower life-cycle cost of the two alternatives. The line segment shown between points "A" and "B" represents a building with a central chiller sized at the minimum capacity that is commercially available. The life-cycle cost between "A" and "B" is not as low as it would be if it were possible to extend the FPFC line to the left of "B" (by using a smaller chiller), represented by the dashed line. However, the oversized chiller alternative still results in a lower life-cycle cost—within the range "A" to "B"—than the PTAC system.

We plan to continue this work by analyzing the effectiveness of other system configurations, operating strategies, and newly developed metering devices. We will also evaluate other building designs and other cities.

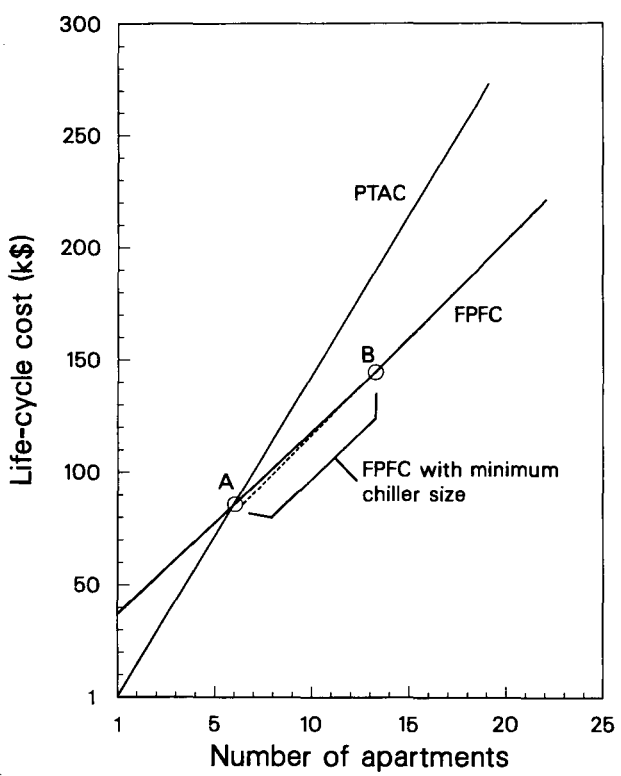


Figure. Life-cycle cost, in Chicago, of central FPFC and individual PTAC with night setback. (XCG-8810-6793)

Analysis of Energy Performance of Unbalanced Single-Pipe Steam Heating Systems in Multifamily Buildings

Y. J. Huang and R. L. Ritschard

For the past two years, LBL has contracted with the Gas Research Institute to analyze the space conditioning loads of prototype multifamily buildings in different U.S. locations (see previous two articles). Roughly 9 million or 40% of all multifamily units are heated by centralized steam or hot water systems, of which nearly half were built before 1940. The great majority of these older units are located in Northeast and Midwest cities, and heated by single-pipe steam systems.

Because this antiquated heating system is prevalent among multifamily buildings, we developed and implemented a simplified simulation model for a single-pipe steam heating system as a modification of the DOE-2.1C program. This model was then used to analyze the energy consumption of older multifamily apartment buildings.

In this simplified model, three new variables were defined: *fill-fraction, mass-heat,* and *anticipator-fraction.* A single thermostat located somewhere in the building controls the steam boiler. The amount of heat delivered to each apartment zone varies according to interactions between boiler capacity, radiator size, and the new variables.

Fill-fraction (see Figure) defines the delay between the time the boiler turns on and when the apartment begins receiving heat. This delay is due to the time needed by the boiler to generate enough steam to displace the cold air in the piping and to heat absorption by the piping mass. *Anticipator-fraction* defines the reduction in maximum heat available to a zone as allowed by the anticipator. By shutting off the boiler, an anticipator reduces the heat output from the radiators even though the thermostat may still be asking for heat. *Mass-heat* defines the residual heat stored or released to the zone hourly by the radiator and piping mass depending on changes in the boiler operating time. The graft shows effects of differing fill-fractions on heat supplied to different apartments.

Simulations were done using this model to analyze energy consumption and indoor temperatures of prototypical pre-1940 buildings heated by single-pipe steam systems under various operational strategies. Sensitivity studies showed that mass-heat would cause typical steam systems without anticipators to overheat from 3° to 6°F and would use 15% to 30% more energy than standard forced-air systems. The effects of three different fill-fractions (none, fast, and slow), anticipator-fractions (0, 10, or 20 minutes), and two thermostat locations were also analyzed. Because of differences in their fill-fractions, top- and ground-floor apartments generally have unbalanced

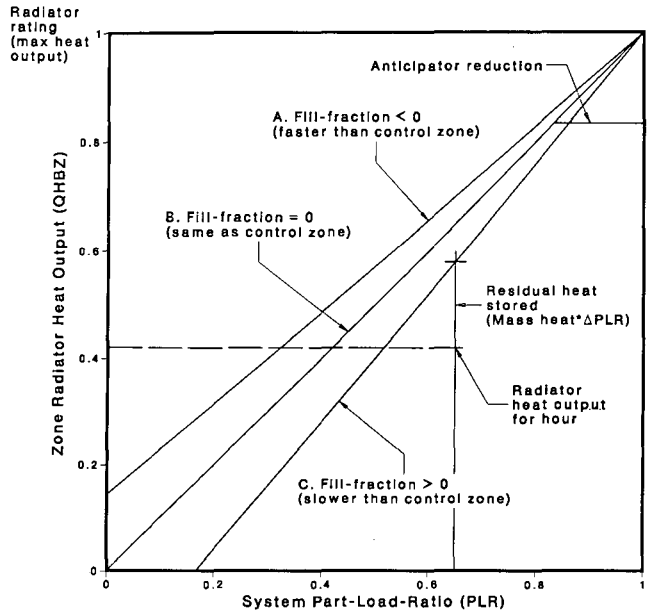


Figure. If a zone's fill-fraction is the same as that for the control zone, the zone receives the same amount of heat (line B in the Figure). If its fill-fraction is greater, the zone will receive heat sooner than the control zone, but the differential disappears as the system part-load-ratio or boiler on-time reaches full load conditions (line A). Conversely, if its fill-fraction is less, the zone receives heat later than the control zone, but the differential again disappears at full-load conditions (line C). The dashed line indicates net heat output into a zone with a slower fill time than the control zone during an hour when ΔPLR is positive and PLR is less than the anticipator-fraction limit. (XBL-8811-3854)

heating and substantially different temperatures. If the thermostat is on the ground floor, the building load is greatly reduced, whereas the top units are underheated.

REFERENCE

1. Huang YJ, Bull JC, Fay JM, and Ritschard RL. *Computer analysis of the energy performance of unbalanced single-pipe steam heating systems in multifamily buildings,* ACEEE 1988 Summer Study on Energy Efficiency in Buildings, Asilomar, CA, 1988.

Estimating Nationwide Conservation Potential From Measured Data

K. Greely, A. Meier, C. Goldman, and J. Harris

Most estimates of regional or nationwide conservation potential have been based on simulated savings derived from engineering models. In contrast, we have developed an approach for estimating conservation potential from measured energy use and have applied this new methodology to two sectors of the U.S. housing stock.[1] Such refined estimates of conservation potential are necessary to accurately assess the extent to which energy conservation has occurred and the amount of savings remaining to be tapped.

Because measured savings have been shown to occur, their use adds certainty to estimates of conservation potential. However, the savings are specific to particular types of retrofits in certain subsectors of the stock. The challenge is to correctly adjust measured savings to compensate for differences between measured projects and the regionwide stock.

The Building Energy Use Compilation and Analysis (BECA) project documents the measured energy performance of new buildings and equipment and the measured energy savings from retrofits. To demonstrate our methodology, we chose two well-documented BECA compilations representing retrofitted multifamily buildings and new, electrically heated, single-family homes.

We first examined the conservation potential of new, electrically heated, single-family homes. We derived savings from construction of efficient new homes by comparing consumption of energy-efficient, electrically heated homes with that of similar "current practice" houses. These savings were combined with estimated construction rates for the next decade to yield a potential energy savings of 0.22 quads per year by 1997 (1 quad = 10^{15} Btu), about 45% of the projected space heating consumption by the new homes. Adjustments were then made to account for differences between new homes in the BECA compilation and the projected stock of new construction, i.e., heating system type, floor area, climate, and energy consumption (see Figure). These adjustments increase the potential energy savings to 0.32 quads per year.

To estimate the conservation potential of existing multifamily buildings in the U.S., we first classified the BECA

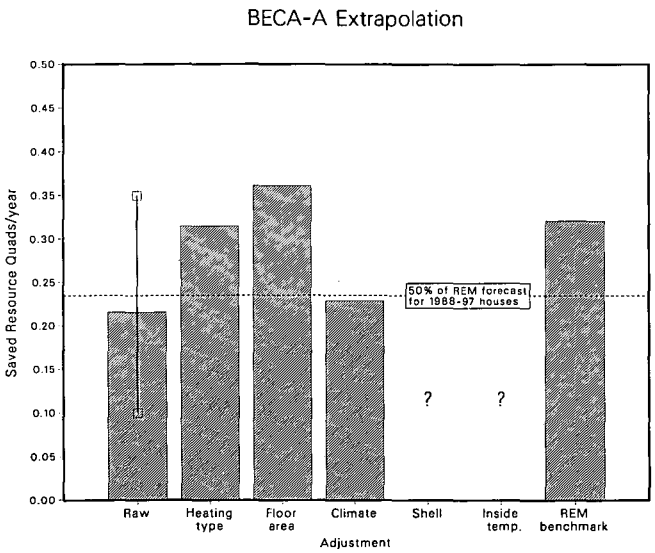


Figure. BECA extrapolation of stockwide savings for new, electrically heated houses. Each bar represents the change in the savings estimate caused by each additional adjustment. "REM" refers to the baseline energy use estimates for new, all-electric homes, from LBL's Residential Energy Model. Adjustments for shell characteristics and inside temperature can be performed as better data become available. (XBL-8811-3855)

multifamily buildings into those with "typical" and "intensive" retrofit packages, segmented by key building and heating system types. Savings for each segment were then extrapolated to the entire multifamily stock, using statistically representative information on consumption and building characteristics of the stock. After adjusting for differences in climate and pre-retrofit usage between BECA buildings and the U.S. multifamily stock, we found that if typical retrofits were installed in all U.S. multifamily buildings, it would save about 0.2 quads per year, while intensive retrofits could save about 0.5 quads per year. These results suggest that current energy consumption in the multifamily sector could be reduced by 9-22%.

We conclude that our method more accurately estimates the conservation potential of a sector than do traditional engineering methods because it is based on measured savings from existing buildings. We plan to improve our methodology through additional adjustments and apply our approach to other sectors of the U.S. building stock.

REFERENCE

1. Meier A, Goldman C, Greely K, Harris J. *Estimating conservation potential using BECA data*, LBL-25126, 1988.

Least-Cost Utility Planning

F. Krause, J. P. Harris, M. D. Levine, and A. H. Rosenfeld

In recent years, a growing number of utilities and state regulatory agencies have adopted a new approach to "integrated" resource planning, aimed at providing customers with *least-cost* energy services through the balanced development of both supply-side and demand-side resources. Technology advances and regulatory reforms have opened up new supply-side options, including renovation of older plants, cogeneration, and power purchases from independent producers. On the customer side of the meter, there are equally exciting new approaches. Utilities, often at the urging of regulatory agencies, are testing new ways to meet customer needs for comfort, heat, light, and power with more efficient end-use technologies. Utility and customer costs can also be reduced by shifting some loads off peak. "Least-cost" utility planning (LCUP) also poses new analytic challenges: to reliably quantify demand-side resources in ways that can be compared with conventional supply-side resources; and to develop integrated utility resource plans that balance economic objectives along with environmental and other policy goals.

In response to a Congressional mandate, the U.S. Department of Energy supports a broad R&D program on least-cost utility planning. LBL's role is to help develop and apply new data and analytical tools to assist utilities and state regulatory commissions in pursuing a balanced, least-cost energy strategy. Most of this effort addresses demand-side opportunities for end-use efficiency and load-shaping, e.g.,

- assess demand-side technologies (performance, cost, reliability, etc.)
- review and evaluate demand-side program experience, including effects of these programs on market penetration of new technologies
- develop and refine analytic tools and models for demand-side analysis and integrated resource planning
- apply new data and analysis techniques to utility-specific studies (see Figure)
- other technology-transfer efforts to encourage use of state-of-the-art planning methods.

Future work will continue evaluation of demand-side programs and technology assessments, collaborative studies with states and utilities, and a special focus on innovative strategies such as utility "resource auctions" for demand-side and supply-side resources.

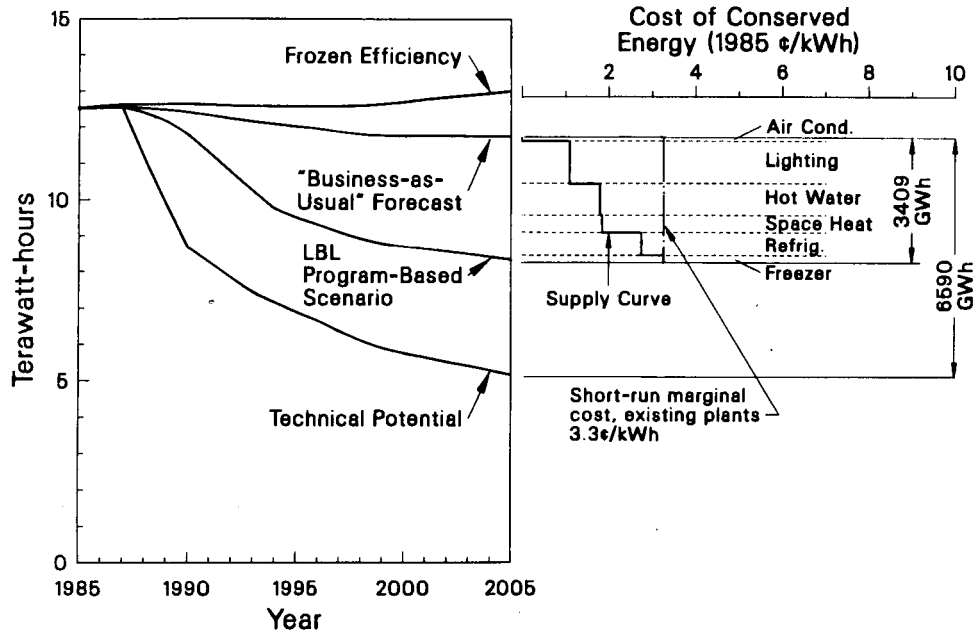


Figure. Graph of Michigan residential electricity use using a conservative "supply curve" to establish technical potential and program scenario. (XCG 881-6508)

Rated vs. Measured Energy Use of Refrigerators

A. K. Meier and K. E. Heinemeier

The energy use of refrigerators is important to both consumers and utilities because they are the largest end use of electricity in most American homes and, together, consume the equivalent electrical output of 25 large power plants. The U.S. Department of Energy (DOE) developed an energy rating procedure for refrigerators. The rated energy consumption was determined through a laboratory test which is the basis for the Energy Guide labels. These labels assist the consumer in selecting the refrigerator with the lowest life-cycle costs, while planning agencies use the energy ratings to forecast electricity demand.

The laboratory test of refrigerator energy use does not attempt to duplicate the actual conditions of a typical refrigerator because they are difficult to determine. Instead, the laboratory test involves measuring the energy use of a refrigerator in a 32°C room, with the door closed, and with no food loads inserted or removed. In spite of these unrealistic assumptions, the energy consumption from the laboratory test has never been carefully compared to field use. In this project, we compared the rated energy use of refrigerators to measured field use.[1]

We collected measured refrigerator use from numerous utility studies and other monitoring programs. The correlation between rated and measured energy use for the 192 units was, on average, excellent (see Figure). However, there was considerable variation among individual refrigerators. This variation was probably due to different operating conditions (especially ambient temperature) and the presence of icemakers, plus random variation in the mechanical performance of individual units.

Monthly energy data were also available for most of the refrigerators. We compared the energy use in the peak and valley months. There was considerable fluctuation in monthly energy use; the maximum and minimum months often differed by more than 30%. These data suggest refrigerators are a greater contributor to the summer electrical peak than previously thought. The results are surprising because most forecasts assume that refrigerators have a nearly constant electrical demand. While the label was quite good at predicting annual energy use, it underpredicted the refrigerator's contribution to the summer peak.

However, for newer (and more efficient) models, the test is less accurate; the rating overpredicted energy use by more than 20% in our sample. This suggests that this type of verification may become even more important in the future.

REFERENCE

1. Meier A, Heinemeier KE. Energy use of residential refrigerators: a comparison of laboratory and field use. *ASHRAE Trans*, 1988; OT-88-14-3.

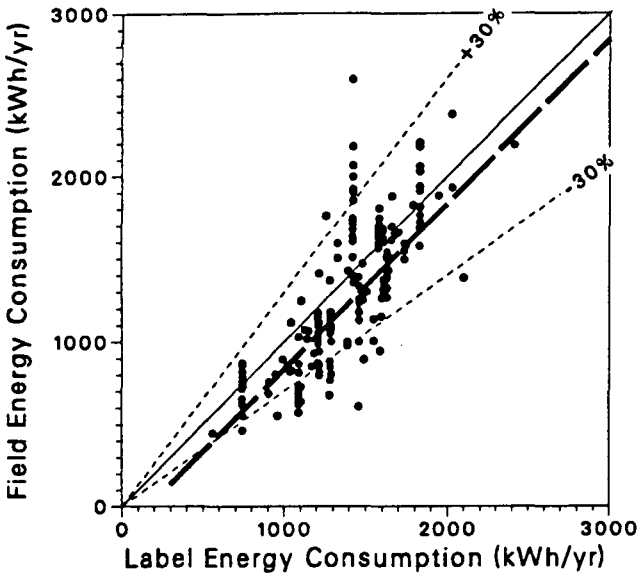


Figure. A scatterplot of DOE laboratory test ("label") consumption versus the measured annual field consumption. A line of perfect agreement is drawn for reference; units to the right of the line represent those with the label consumption greater than the field consumption. On average, the field consumption was very close to the rating, although individual models show some scatter around the line of agreement. The "columns" of points represent groups of identical refrigerators. (XBL-8810-3619)

Experience with Energy Efficiency Programs for New Buildings

E. Vine and J. Harris

This report evaluates the experience with implementing programs promoting energy efficiency in new residential and commercial construction. This report is one of a series of program experience reports that seek to synthesize current information from both published and unpublished sources to help utilities, state regulatory commissions, and others to identify, design, and manage demand-side programs.

We focused our investigation on nonregulatory programs that are designed to complement—or in some cases substitute for—mandatory energy efficiency requirements in local and state building codes. We evaluated the following types of nonmandatory programs: technology demonstrations and demonstration programs, financial incentive programs (including rebates, conservation rates, reduced hookup fees, reduced rates on loans and loan qualifications, guaranteed savings, and tax credits), consumer information and marketing programs (including energy rating systems and energy awards), technical information programs (including professional guidelines, design tools, design assistance, and standards-related training, compliance, and quality control), and site and community planning.

In addition to presenting findings for each program category, we summarize general program conclusions, applicable to most of the energy conservation programs reviewed in this report: (1) many different types of nonmandatory programs appeared to be successful in overcoming barriers to promoting energy efficiency in new buildings; (2) no program strategy was clearly dominant; (3) few program evaluation studies exist, resulting in a paucity of quantitative data on program effectiveness, especially beyond the pilot or demonstration stages; (4) only a few programs were designed as part of a long-term strategy to promote energy-efficient construction; (5) successful programs were often characterized by intervention early in the design and planning process in order to minimize delays in the project design, approval, financing, and construction process; (6) education, training, and design assistance activities were especially important; (7) most programs focused on the early design stages of a program without addressing issues normally arising later in the program (e.g., details of construction, quality control, building commissioning, and operations and maintenance); (8) utility rate designs were typically not used as conscious reinforcement for promoting energy-efficient construction; (9) many programs were considered successful for both energy and nonenergy reasons (e.g., improved thermal comfort, creation of new markets, and improved customer relations); (10) nonmandatory programs can reinforce and pave the way for codes; and (11) most of these programs can be easily implemented in other areas around the country and in other countries.

For the design and implementation of energy conservation programs for new buildings, the evidence suggests that a comprehensive and long-term perspective is needed to design and choose programs. Long-term goals and objectives of programs need to be made explicit in order to provide program guidance. A well-integrated package of programs should contain the following program strategies: design assistance, financial incentives, quality control, training and education of design professionals and the building community, simple and easy-to-use design tools, rating and labeling of buildings, effective marketing and promotion, energy awards for buildings and for design and building professionals, building commissioning, operations and maintenance activities, process and impact evaluation, monitoring, and feedback activities.

Implementation of energy efficiency programs is not an easy task, and there have been many failures at various stages in the implementation process. The challenge is to design and implement a program that meets the needs of the target audiences as well as promote energy-efficient construction.

Analysis of Commercial Electric End-Use Data

H. Akbari, I. Turiel, J. Eto, and L. Rainer

Direct metering is the most expensive method for gathering reliable load shape data on electrical end uses. The goal of this project, which was jointly sponsored by the Southern California Edison Company (SCE) and the California Energy Commission, is to investigate a less expensive alternative to metering using 15-minute interval whole-building electric loads. Successful development of such an alternative could reduce the cost of obtaining high quality load shape data by several orders of magnitude. Given the stakes involved in electric utility resource planning, the returns promise to be large.

Our approach is to conduct detailed analyses of SCE data on commercial building characteristics, energy use, and whole-building load shapes, and in conjunction with other data, to develop, test, and apply an integrated method to estimate end-use load shapes (LSs) and energy utilization indices (EUIs). The primary data for the project are on-site surveys, load research data (LRD), and available sub-metered energy use data. Secondary data include other EUI and LS studies, commercial sector mail survey data, and typical and historic southern California weather data.

The project consists of two major parts: the first concerns the development of prototypical buildings and the performance of energy use simulations that lead to preliminary estimates of LSs and EUIs. This part relies primarily on survey data, which are complemented by results from previous EUI and LS studies. The second part entails selective modification of the initial estimates using whole building load research and historical weather data. The methodology is illustrated schematically in the Figure.

Development of a Simplified Tool to Calculate Commercial Sector EUIs

I. Turiel and B. Lebot

This project, supported by the Electric Power Research Institute (EPRI), developed a simplified tool to calculate commercial sector energy utilization indices (EUIs). In EPRI's Commercial Sector End-Use Planning System (COMMEND) model, EUI values are one of the three key market facts. Together with floor stock and market share data, EUI values allow the construction of market profiles that depict energy use patterns at the end-use level. These profiles are important for analysis of the current energy market and they provide a starting point for end-use forecasting. The computer software developed in this project allows utilities to calculate EUIs specific to their

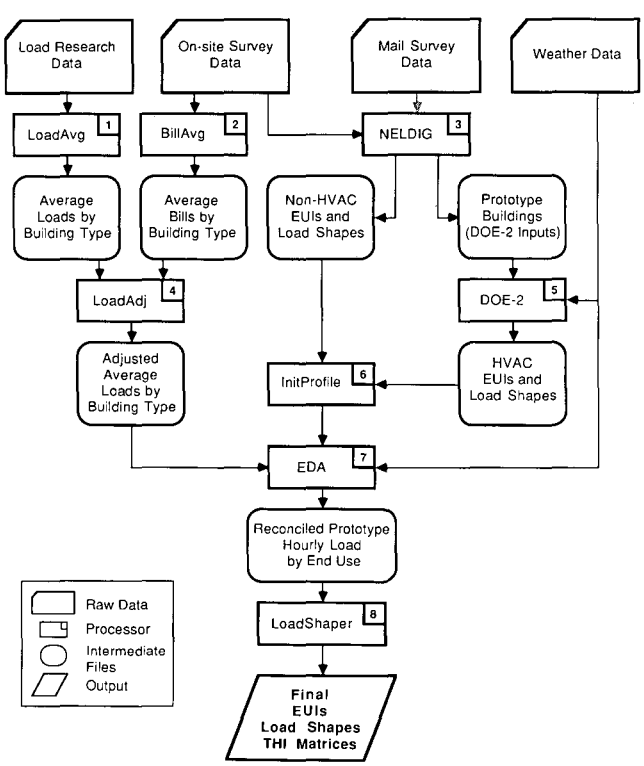


Figure. Integrated LS and EUI Estimation Methodology: The methodology has four major steps: 1) development of initial prototypical LSs and EUIs, using the on-site survey and mail data. Two utility programs, Non-HVAC EUI/LS and DOE-2 Input Generator (**NELDIG**) (estimates LSs and annual EUIs for non-HVAC end uses and prepares prototypical building input data for DOE-2 simulations) and initial profile generator, **InitProfile** (combines DOE-2 and NELDIG outputs to prepare initial estimates of hourly end-use loads), are used for this purpose; 2) construction of average hourly loads for prototype buildings using the monthly billing data and load research data. Three programs are developed for this second process: **BillAvg** (computes the average utility bills by building type from the on-site survey billing data), **LoadAvg** (computes the average hourly whole-building loads by building type from LRD), and **LoadAdj** (computes the average hourly whole-building load as normalized by average utility bills); 3) reconciliation of the initial end-use data from the first step with the average hourly loads from the second step using the End-use Disaggregation Algorithm (**EDA**); and 4) summarizing the reconciled hourly end-use data in the form of representative monthly load shapes, using a program called **LoadShaper**. (XBL-8811-3881)

service area without undertaking extensive studies such as a conditional demand analysis or end-use metering.

Two approaches were used to develop the EUI specifications for each end-use and business type combination studied. First, previously published EUI studies for the commercial sector were analyzed. An averaging procedure of selected studies yielded the non-weather-sensitive EUIs. Second, the 1979 Nonresidential Building Energy Consumption Survey data set was used to estimate weather-sensitive EUIs. A conditional demand analysis performed with this data set obtained heating and cooling EUIs as a function of building characteristics, operating conditions, and climate parameters.

The end products of this project are a spreadsheet program, a users guide, and an EPRI report.[1] The spreadsheet program, developed with the Lotus 123® software, calculates a matrix of EUIs for eight electrical end-uses for eleven building types. The Figure shows the flow diagram describing how the spreadsheet works. Any utility using this tool can either provide input data specific to the commercial buildings in their service territory or, in the absence of such information, use the default data provided in the software for their census region. The program also allows the user to plot bar graphs of EUIs by building types. The report provides comparisons between the EUI predictions of the program with those EUIs estimated in several electric utilities' conditional demand studies.

The spreadsheet will be used nationwide by utilities already using the COMMEND model. Several improvements have been proposed to the existing program, such as adding sensitivities of the EUIs to new parameters and adding algorithms to calculate EUIs for natural gas use.

REFERENCE

1. Turiel I, Lebot B. *Development of a simplified tool to calculate commercial sector EUIs*, draft report to EPRI, 1988.

Comparative Assessment of the DSM Plans of Four New York Utilities

C. Goldman and E. Kahn

In April 1988, New York's seven investor-owned utilities filed their first long-term Demand Side Management (DSM) Plans in response to a Public Service Commission (PSC) order. The PSC invited LBL researchers in DOE's Least Cost Utility Planning project to assist Commission staff in reviewing the utility's long-term demand-side resource plans. The principal research objective was to identify the most important least cost utility issues facing public utility commissions based on actual experience gained from working with commission staff.

Comparing the DSM plans of four utilities—Consolidated Edison, Niagara Mohawk, New York State Electric and Gas, and Rochester Gas and Electric—we assessed the potential impact of DSM programs among utilities by the year 2000 (Table). The initial DSM plans of all four utilities are modest in terms of the contribution of DSM options to reducing total system peak load in the year 2000 (3-7%). Expected savings from DSM programs range between 0-50% of the peak load growth projected for that period. However, we believe that the key indicator is "utility commitment," which reflects the utilities' stated willingness or actual commitment of dollars to implement new large-scale DSM programs in the near-term. Several utilities believe that the uncertainties associated with DSM programs are too high to justify major investments.

All four utilities identify commercial lighting as an end-use with cost-effective DSM options. Of the four utilities, only Con Edison identifies other DSM options applicable to commercial buildings (e.g., motors, thermal cool storage, efficient air conditioning replacement, curtailable electric service). In the residential sector, the summer

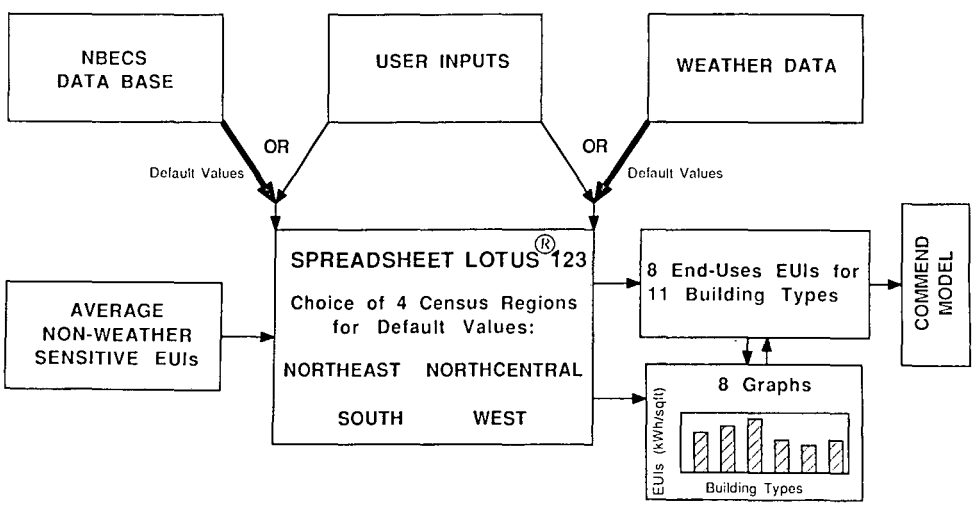


Figure. Flow diagram describing how the spreadsheet works. (XBL-8810-3741)

Table. Potential impact of demand-side management programs

	1987 Peak Load (MW)	Projected Load Growth to 2000 without DSM	DSM Impact Indicators: Peak Load Reduction due to DSM (MW)	% of Peak Load Growth	% of Peak Load	Utility Commitment[a]
Con Ed	9400	2092	742	36%	6.9%	A
RG&E	1205	255	0-105	0-41%	0-7.5%	P
NYSEG	2477	769	116	15%	3.6%	A
NiMo	5800	500	0-250	0-50%	0-4.0%	P

Con Ed and RG&E are summer peaking; NYSEG and NiMo are winter peaking utilities.
[a] P = planned; A = action on some programs

peaking utilities (Con Ed and RG&E) found that replacing existing room air conditioners with high-efficiency equipment and peak clipping measures (e.g., direct control of room air conditioners and pool motors) were cost-effective DSM options. Winter-peaking utilities (NYSEG and NiMo) favored load-shifting DSM options (e.g., direct control of water heating and residential thermal storage).

We also identified the most important data and analysis needs for regulators trying to evaluate DSM plans: improved stock characterization, explicit treatment of Qualifying Facilities (QFs) in resource mix, comprehensive assessment of the achievable potential for DSM options for all end uses and sectors, research on customer response and other information relevant to DSM options (load shape impacts, incentives required to achieve certain penetration rates), and projections of avoided costs. More reliable data are available on DSM options for the residential sector than for the commercial and industrial sectors.

Our analysis also suggests that the PSC and utilities must resolve several thorny analytical and methodological problems that hinder DSM program implementation. For example, the utilities used varying economic tests for initial screening and final selection of DSM options. The PSC may need to develop a more explicit treatment of the role of various economic tests in DSM program evaluation. In addition, the utilities were particularly concerned that DSM programs would lead to substantial near-term revenue losses. Thus, the timing of DSM programs is a particularly critical issue: programs and incentives should be selected that meet the twin goals of minimizing short-run negative rate impacts while preparing for long-run expansion of DSM programs. Finally, because New York utilities are members of a centrally-dispatched power pool, DSM options should be evaluated from the perspective of optimizing benefits for the New York Power Pool. Several utilities are assessing the costs and benefits of DSM options from their individual perspectives only; for winter-peaking utilities, this approach understates the benefits of DSM measures that could reduce the Power Pool's summer peak load.

REFERENCE

1. Goldman C, Kahn E. *Review of the Demand-Side Management Plans of Four New York Utilities*, LBL-26374, 1988.

Energy Use and Efficiency of Electronic Office Equipment

J. P. Harris

Electronic office equipment, including personal computers (PCs), minicomputers, printers, copiers, fax machines, etc., represents a fast-growing but poorly understood component of the "other" end-use in commercial buildings. This study attempts to establish office electronics as a distinct end-use, by characterizing electricity usage, trends, and efficiency opportunities. We can think of this equipment as the office equivalent to industrial process equipment; in office buildings the main "process" is the production, use, storage, and transmission of information. Except for space conditioning and lighting, information processing is the major user of energy in office buildings (up to 20% of total daytime electricity use).

Typical daytime loads from office equipment (10-20 W/m^2) are about equal to lighting loads in a well-designed new office. We measured actual power use for selected office equipment, and found that it was only 20-40% of nameplate ratings. Thus, estimates of energy use

or cooling loads based on nameplate ratings are overstated. Power use varies widely for office equipment with similar functions. In particular, desktop PCs use about ten times the power of equivalent laptop models. It is often the input/output (I/O) devices (terminals, printers, scanners, fax), rather than computers themselves, that are the major power users. Future load growth depends on many market and technical factors. U.S. office equipment electricity use in 1995 could range from 130 TWh ("market saturation," current technology, expanded use of computerized printing), to about 25 TWh if today's most efficient hardware and operating systems become the norm (see Figure).

There is significant potential for improved energy efficiency in both hardware and software. Several policy options could accelerate market and technical trends (e.g., miniaturization, portability). Examples include energy efficiency labeling of hardware and software, and creative use of government purchasing power. In the longer term, better-integrated information management systems may finally introduce the "paperless office," with major impacts on both energy use and office productivity.

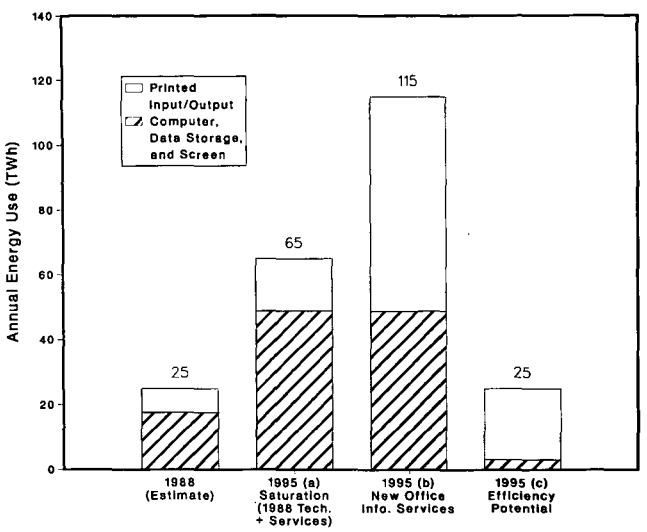


Figure. Alternative load growth scenarios for office electronic equipment in the U.S. The 1988 estimate is based on 25 million "screens" serving 60 million white-collar workers, averaging 200 W/user (equivalent to a PC workstation or shared mini- or mainframe, plus screen and peripherals) and 5000 hours/year operation. The 1995(a) scenario assumes today's hardware efficiencies and usage, with full "market saturation" (65 million screens). The 1995(b) scenario shows the impact of new information services, e.g., increased I/O using computer-generated or -scanned hard-copy. Power requirements for I/O increase from 50 to 200 W/user, nearly doubling total energy use. The 1995(c) scenario ("technology potential") assumes universal adoption of today's most efficient hardware and operating systems. This reduces power from 150 to 15 W/user for computers, and from 200 to 100 W/user for I/O. Better control of idle-time would reduce average operating time to 3000 hours/year, bringing total U.S. electricity use for office electronics back to today's 25 TWh. (XBL-8810-3602)

REFERENCE

1. Norford L, Rabl A, Harris J, Roturier J. *Electronic office equipment: The impact of market trends and technology on end-use demand for electricity.* LBL-25558, 1988. (Forthcoming 1989, Proceedings of the Vattenfall Electricity Congress, Gothenberg, Sweden.)

EMCS for Utility/Customer Interface

H. Akbari, M. Goralka, and K. Heinemeier

Energy Management and Control Systems (EMCS) are being installed at an accelerating rate in new and retrofitted commercial buildings. We have explored the capabilities of EMCS for use as an interface between electric utilities and their customers for both real-time pricing and end-use data monitoring of commercial buildings. Our research, sponsored by the Pacific Gas and Electric Company, indicates that currently-sold EMCSs are intelligent enough to perform these applications, but lack the necessary software communication features and installed metering capacity for any large-scale effort with real-time pricing or data monitoring.

We have demonstrated the feasibility of the above goals by 1) performing a detailed review of previous LBL studies that demonstrate the concept of remotely collecting data from EMCSs, and 2) conducting a real-time pricing simulation.[1] From these demonstration projects, we developed specifications recommending the necessary EMCS system hardware and software features which could be incorporated into current EMCS.

Typical EMCSs sold today are fundamentally different from machines sold just four to five years ago. A typical large EMCS (see Figure) has three components: a local control module (LCM) which is directly wired to the sensors and relays, a field processing unit (FPU) which makes control decisions, and a personal computer interface. An important feature of the typical system is its modularity. The most powerful EMCS installations have all three components, but often only a FPU or a LCM is necessary for more limited applications such as controlling a single air conditioning unit. Thus, each of these components is capable of stand-alone operation without the other, higher level, components.

The utility's main interest in commercial monitoring is to obtain end-use data for forecasting commercial energy consumption and estimating how this consumption can be predictively modified to decrease the utility's net cost of

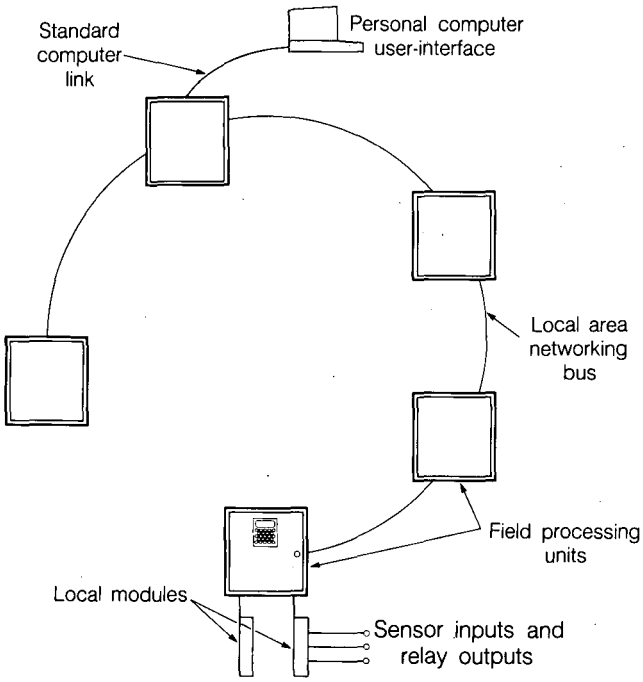


Figure. Architecture of a typical large EMCS. A typical large EMCS has three components: a local control module (LCM), a field processing unit (FPU), and a personal computer interface. (XBL-8810-8581)

services or enhance revenues. Performing this analysis requires end-use intensities and load-shape data for use in utility planning. Utilities use these data in their long- and short-term energy and peak demand forecasts, conservation and load management assessments, marketing assessments of the best end-uses to sell, capacity planning for transmission and distribution, cost-of-service/rate design for profitable end-uses, and modeling the effects of fuel substitution.

EMCSs could easily provide the information required for these analyses. Some modifications of the current systems would be required, however. If these modifications can be accomplished, a wealth of information would be available to a utility. A significant fraction of all commercial buildings already have EMCSs installed to control their HVAC equipment. The data collection process would involve a communications link, where either the EMCS automatically downloads data to a utility over a phone modem, or a utility calls up the EMCS for interrogation of the data.

The use of EMCSs in commercial buildings under real-time pricing would enable customers to adjust their demand automatically in response to fluctuating prices. The process would involve establishing a communications link between the utility and the customer's EMCS. Once a day, the utility would send an hourly price schedule to the building's EMCS. The EMCS would then use the price data to automatically instigate control strategies intended to minimize energy consumption during hours with high prices. In this way, the customer can minimize energy bills with a minimum effort and the utility will see a reduced demand during peak periods and other times when power is most expensive to produce.

REFERENCE

1. Heinemeier KE, Akbari H. Capabilities of in-place energy management systems for remote monitoring of building energy performance: case studies. *ASHRAE Trans.*, 1987; NT-87-28-1, 93(2):2321-2336.

Field Measurement of Heat Island Data

H. Akbari, L. Rainer, and H. Taha

Although the existence of urban heat islands has been known for many years, actual measured microclimate data to quantify this effect has been limited. There has been little simultaneous multiple-site measurement of microclimatic data over long time periods. These long-term data are required to validate and improve the numerical models for predicting the impact of heat islands on cooling energy use.

Two major field studies, one in Davis, CA and one in Sacramento, CA, were carried out by the "Heat Island Project" at LBL.* Both studies have yielded valuable heat island data.

In the Davis project, a well-defined tree canopy (i.e., an orchard) surrounded by open space was transected with eleven weather stations that measured dry-bulb and dew-point temperatures, wind speed, and wind direction at 1.5m above the ground. Data were collected at fifteen-minute intervals for two weeks starting on October 12, 1986. The main objective was to quantify the effects of vegetative canopies on micro-climates and in particular their creation of an oasis effect during daytime. Data were studied to analyze the variation of air temperature and wind speed within the canopy. Figure 1 shows a typical daytime air temperature traverse across the orchard. On average, the canopy was about 2°C cooler than the open fields.

Whereas the Davis project dealt with microclimatic changes within a single orchard with a grid spacing of ~100 m, the Sacramento project attempted to extend this measurement to a whole city with a grid spacing of ~1 km. In this study, the weather stations were distributed throughout Sacramento in 15 residential locations with a

*This work was supported in part by a grant from University-wide Energy Research Group, University of California, Berkeley.

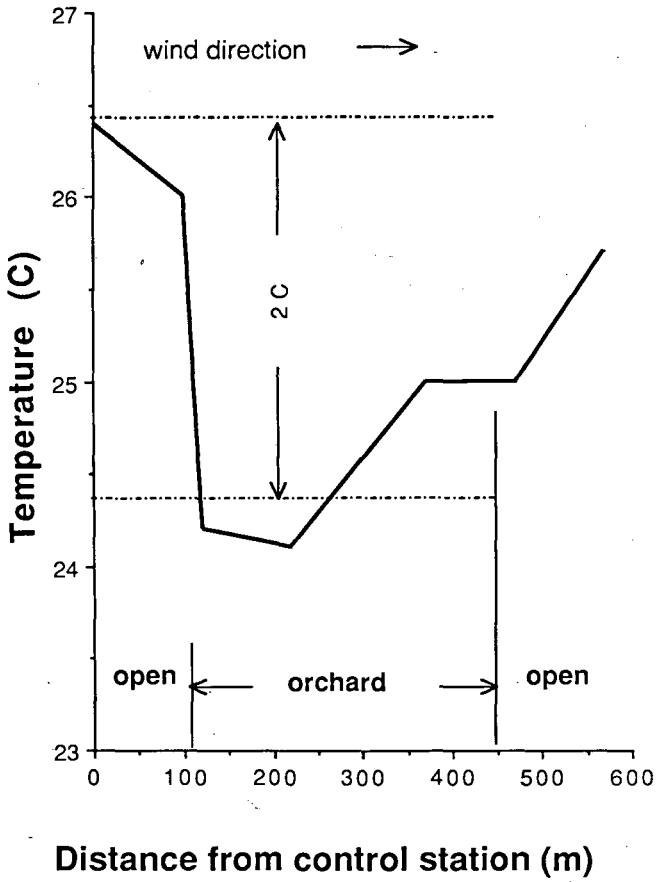


Figure 1. The average effect of trees on the drybulb temperature at 3 PM during October 1986 in Davis, CA. (XBL-8811-3895)

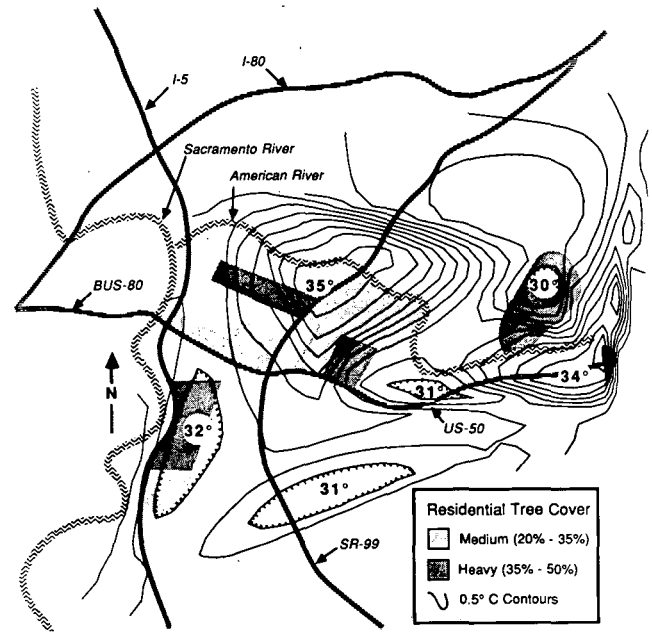


Figure 2. Heat island temperature contours at 4 PM on August 5, 1987 in Sacramento, CA. (XBL-8812-4076)

variety of tree cover. Half-hourly data were recorded for each of these sites from July 16 through September 19, 1987. Additional weather data, including cloud cover, were collected using a computer weather monitoring network located at four local airports.

The Sacramento data have been analyzed in two ways. First, they were analyzed to quantify the effect of local characteristics such as tree cover and skyview factor on the local climate. Regression equations were then developed relating inter-site temperature differences to these local characteristics and daily weather factors such as temperature, wind speed, and wind direction. Secondly, the data were analyzed to extract an overall picture of the summer heat island and its changes throughout the day. As an example, Figure 2 shows the temperature contour on a hot August day. The temperature varies from 35°C downtown to 30°C in some of the outlying neighborhoods. Further analysis of the data shows that heavy tree cover can reduce the effect of urban heat islands by as much as 3°C.

Analysis of Residential End-Use Load Shapes

H. Ruderman, J. H. Eto, K. E. Heinemeier, A. Golan, and D. Wood

Over the past ten years, the California Energy Commission (CEC) has developed models to forecast electricity demand and peak loads in the state.[1] The models use individual end-use daily load shapes to calculate hourly loads on peak days for both weather-sensitive and non-weather-sensitive end uses. Our project, sponsored by the CEC, analyzes available metered data on end-use load shapes to refine the current estimates used in the CEC peak demand models. Initial emphasis has been placed on residential loads because of data availability; future work will concentrate on non-residential end uses. The project will also assist the Commission in laying the groundwork for transforming their peak demand models into models that forecast hourly loads throughout the year, relying on LBL's experience in constructing and validating its Residential Hourly and Peak Load Model.[2]

Since the project began in the summer of 1987, we have collected metered residential end-use data from the three largest electric utilities in California. End uses were

classified as conditioning (space heating and cooling) or non-conditioning (water heating, cooking, refrigeration, etc.); each group was analyzed by different techniques. For non-conditioning end uses, we aggregated the metered data into monthly and seasonal energy consumption profiles and then constructed daily load profiles for weekdays and weekend days for each season (see Figure). For conditioning end uses, we constructed matrices showing average load as a function of time of day and of outdoor temperature (or temperature-humidity index). We devised a new fitting procedure to describe the average load as a function of time and temperature suitable for use in residential load models. To our knowledge, ours is the first analytic expression developed to describe the behavior of space conditioning equipment. A final report to the CEC describing data sources, analytic methodology, and results will be written in FY 1990. Revised load shapes will be incorporated in the LBL Residential Hourly and Peak Load Model.

REFERENCES

1. California Energy Commission. *California energy demand: 1985-2005, Volume II: Electricity demand forecasting methods,* CEC Publication No. P300-87-004, Sacramento, CA, 1987.
2. Verzhbinsky G, Ruderman H, Levine, MD. *The residential hourly and peak load model: description and validation,* LBL-18698, 1986.

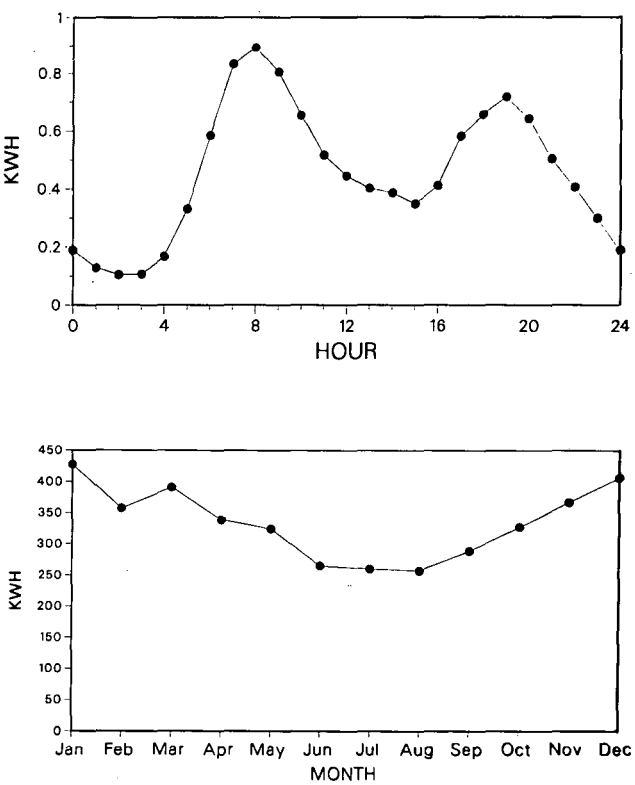


Figure. Average daily and monthly load shapes for water heaters. (XBL-8810-3589)

Analysis of Federal Appliance Efficiency Standards

H. Ruderman, P. Chan, P. Cunliffe, A. Heydari, J. Hobart, J. Koomey, B. Lebot, M. D. Levine, J. E. McMahon, T. Springer, S. Stoft, I. Turiel, and D. Wood

In March 1987, Congress passed and the President signed the National Appliance Energy Conservation Act (NAECA)[1] establishing efficiency standards for household appliances. The legislation provides for periodic update of the standards by the Department of Energy. LBL is responsible for an integrated analysis of the impacts of these appliance efficiency standards. The research involves a detailed assessment of the impacts on consumers, manufacturers, electric utilities, and on the nation as a whole. Work during FY 1988 focused on providing analytic support for DOE's rulemaking on two groups of products: (1) refrigerators, freezers, small gas furnaces, and television sets; and (2) dishwashers, clothes washers, and clothes dryers.

Our analysis has four major components: (1) an Engineering Analysis to quantify the efficiency improvements of various design options and their costs; (2) a Consumer Analysis to project the energy use, shipments, purchase price, and operating costs of more efficient products; (3) a Manufacturer Analysis to determine impacts on the appliance manufacturing industry; and (4) an Impact Analysis to examine the impacts of standards on various groups. The latter analysis includes changes in consumer life-cycle costs, competition within the manufacturing industry, fuel savings and reduced need for new generating capacity by electric utilities, an assessment of environmental impacts, energy savings by fuel type, and the net present benefit of standards to the nation. The Figure shows how the parts of the analysis are interrelated and how they fulfill legislative requirements for evaluating the impacts of standards. The following three articles provide more detailed information on how the Engineering, Consumer, and Manufacturer Analyses are performed.

The analysis of standards on refrigerators, freezers, small gas furnaces, and television sets was completed in the first quarter of FY 1988. We documented the methodology and results of the analysis in the Technical Support Document[2] published by DOE with their Notice of Proposed Rulemaking. Major improvements were made in the utility and environmental parts of the Impact Analysis for refrigerators and freezers. The utility analysis evaluated avoided utility costs, lost revenues, and generating capacity deferrals that would result from imposition of standards. In addition to estimating the reduction of power plant emissions, the environmental assessment examined changes in chlorofluorocarbon use in these appliances. We also focused on the competition between electricity and gas in the small furnace market.

To analyze the impacts of possible amended standards for clothes washers, clothes dryers, and dishwashers, we collected data on the cost and efficiency of design options

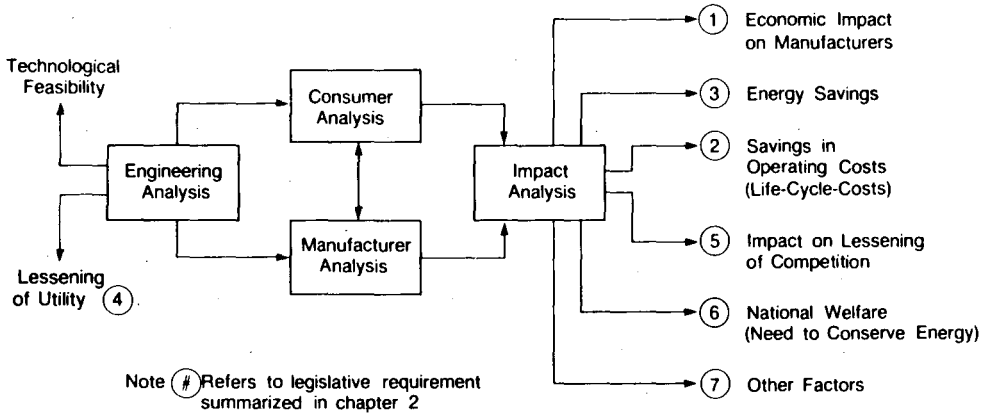


Figure. Satisfaction of legislative requirements through the analysis process. (XBL 856-8918)

for improved efficiency of these products. We modified the LBL Residential Energy Model to take into account changes in water heater energy consumption when the efficiency of clothes washers and dishwashers is increased. Analysis of these three products will continue in the first quarter of FY 1989, emphasizing the estimated reduction in water use and the cost of water and waste treatment that would occur if certain design options were employed.

REFERENCES

1. *National Appliance Energy Conservation Act*, Public Law 100-12, March 17, 1987.
2. U.S. Department of Energy, Assistant Secretary for Conservation and Renewable Energy, Building Equipment Division, *Technical support document: energy conservation standards for consumer products: refrigerators, furnaces, and television sets*, DOE/CE-0239, report prepared by Lawrence Berkeley Laboratory, November 1988.

Engineering Analyses of Appliance Efficiency Improvements

I. Turiel, A. Heydari, and B. Lebot

The economic impacts of appliance efficiency standards depend largely on the relation between cost and energy consumption of a consumer product. Our engineering analysis seeks primarily to identify this cost-consumption relation for selected appliances. In FY 1988, we analyzed refrigerators, freezers, televisions, small gas furnaces, dishwashers, clothes washers, and clothes dryers, addressing two legislative requirements: to estimate the maximum technologically feasible efficiency levels that are possible and to ensure that new designs do not lessen consumer utility.

Our analysis selects appliance classes, baseline units, and design options, determines maximum technologically feasible designs and the efficiency improvement provided by each option, develops cost estimates, and generates price-efficiency relationships. We have studied 10 classes of refrigerators and freezers, as well as two classes each of televisions, small gas furnaces, dishwashers, clothes washers, and dryers. Many design options were studied for each product class[1]. For refrigerators and freezers, a computer simulation model was used to estimate energy use under different design options. We also evaluated the energy consumption impact caused by using only those design options that did not increase the baseline amounts of chlorofluorocarbons (CFCs).

We developed energy consumption data for other products by using test data from various sources, manufacturer-provided data, and engineering calculations. Manufacturer costs were obtained from data submitted by manufacturers and from component suppliers. These costs were disaggregated into labor, materials, purchased parts, tooling and capital costs, and shipping and packaging.

The results of the simulation analyses for a top-mount automatic-defrost refrigerator-freezer are shown in the Figure. Simulations were performed under two scenarios. The cross-hatched bars in the Figure show energy use for design options which allow the amount of CFC-11 to increase above that in the baseline case unit. The white bars exclude options 2, 6, 9, and 10, which require increases in CFC-11.

In FY 1989, we plan to complete the engineering analysis for dishwashers, clothes washers, and clothes dryers. We will also evaluate other design options such as higher spin rpm for clothes washers, simultaneously considering washers and dryers in order to compute benefits. We will also respond to public comments on Notices of Proposed Rulemaking.

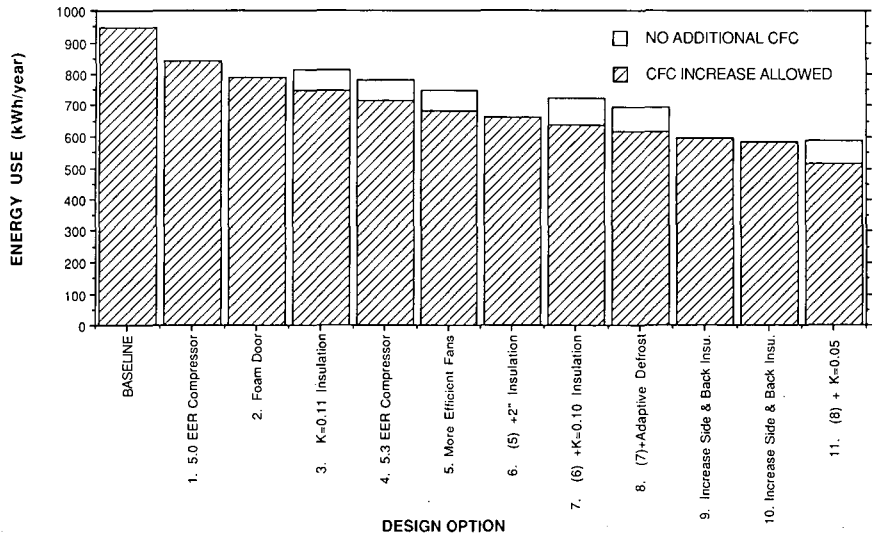


Figure. Energy use of a top-mounted auto defrost refrigerator-freezer for various design options (adjusted volume = 20.8 cu.ft). (XBL-8810-3614)

REFERENCE

1. Turiel I. *Design options for energy efficiency improvement of residential appliances,* LBL-22372, 1986.

Assessment of Impacts of Appliance Standards on Manufacturers

S. Stoft, P. Cunliffe, and J. Hobart

The Manufacturer Analysis determines the impact of appliance standards on the the profitability and competitiveness of the various appliance manufacturing industries. It also provides estimates of retail prices that are used by the Residential Energy Model (LBL-REM) and the life-cycle cost analysis. The Manufacturer Impact Model (LBL-MIM) uses engineering cost and efficiency estimates as well as economic and financial data that we collect to generate the necessary predictions for this analysis. Besides price and rate of profit, these include shipments, revenues, and net incomes, as well as standard errors on of all these.

In the first half of FY 1988, we completed the new version of the LBL-MIM and automated its running. It now does all of the Monte Carlo calculations, scenario evaluation, and production of tables for the Technical Support Document (TSD) automatically. After completion, it was used to analyze impacts of possible standards on the manufacturers of refrigerators, freezers, televisions, and small gas furnaces, and to produce the appropriate tables for the TSD. In general, LBL-MIM showed that approximately all increases in manufacturing cost would be passed on by manufacturers to consumers. For some standards levels, markups were observed to increase slightly, causing an increase in profits, while for other levels a decrease in profits was observed.

During the second half of FY 1988, one major improvement was made which affects the Manufacturer Analysis and, once it has been fully extended to LBL-REM, will allow greater compatibility between LBL-MIM and LBL-REM. This involved changing the demand specification from one that implies constant price elasticity to one that implies constant life-cycle-cost elasticity. Consequently, the price elasticity now changes slightly as both the price and operating cost of an appliance change. Since price elasticity determines the manufacturer's markup, these elasticity effects, though small, can have a significant effect on a manufacturer's profits.

We also collected data on the dishwasher and laundry products industries. This included a survey of the industries, developed by us and administered by AHAM, a meeting with consultants from the dishwasher industry, and a visit to a major manufacturer. Finally, we completed our initial analysis and the initial draft of the TSD for these products.

Residential Energy Demand Forecasting

J. E. McMahon and P. Chan

The LBL Residential Energy Model (LBL-REM) provides estimates of the impacts on consumers of federal policies affecting energy consumption by home appliances, including furnaces and air conditioners. LBL-REM combines engineering estimates of possible appliance designs with a simulation of market behavior for the purchase of appliances, including fuel choice, efficiency choice, and usage behavior (see Figure).

The LBL-REM has been improved this year by: incorporating the effects of the National Appliance Energy Conservation Act (NAECA) of 1987 into the base case; modeling the interactions between internal loads (e.g., waste heat from refrigerators) and space conditioning energy use (heating and cooling); directly using discrete design options from engineering analyses, without any smoothing or curve fitting (new data became available for refrigerators, refrigerator-freezers, freezers, and some new sub-markets listed below); and explicitly modeling the individual sub-markets for small gas furnaces, dishwashers, clothes washers, and televisions (none of which were previously analyzed).

The model was used to perform several analyses of impacts of federal policies on consumers and on national energy consumption, including: regional impacts of the NAECA; possible new conservation standards for small gas furnaces, televisions, and dishwashers; and possible updates to conservation standards for refrigerators, refrigerator-freezers, freezers, clothes washers, and clothes dryers.

In addition, LBL-REM results were used to analyze impacts on manufacturers, electric utilities, and the environment.

We plan to continue to model impacts of any proposed federal conservation standards, including incorporating into LBL-REM any new data from public comments on the proposed rules for dishwashers, televisions, and small gas furnaces, and on updated standards for refrigerators, refrigerator-freezers, freezers, clothes washers, and clothes dryers. A new water heater algorithm will be formulated to take into account hot water use by clothes washers and dishwashers. A new feature will be estimates of impacts of federal energy conservation standards on residential water consumption and on water and sewage costs. The future analysis of room air conditioners, water heaters, direct heating equipment, and pool heaters will be performed on a regional basis. We will continue improving the consumer analysis and forecasting capabilities of LBL-REM.

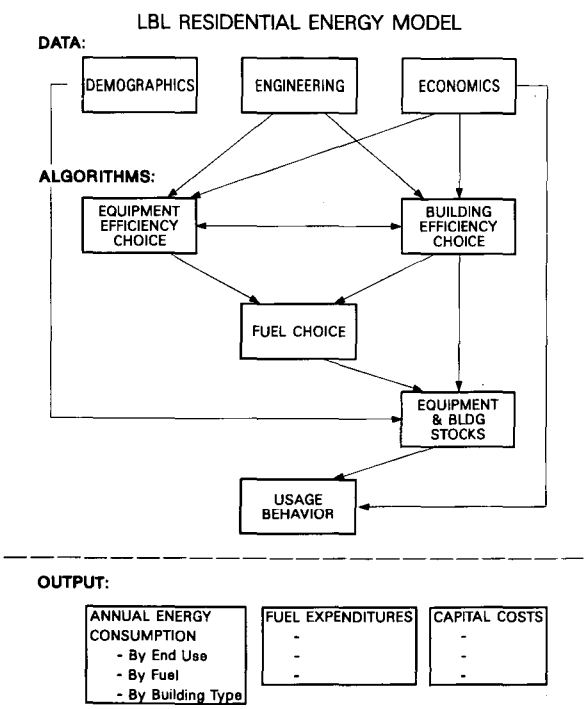


Figure. Logic diagram showing major components of LBL Residential Energy Model. (XCG 8412-13510)

The Regional Energy and Economic Impacts of Appliance Efficiency Standards

J. H. Eto, J. E. McMahon, J. G. Koomey, P. T. Chan, and M. D. Levine

While nationwide analyses performed by LBL overwhelmingly support the cost-effectiveness of appliance efficiency standards, the regional impacts of the standards have never been examined. These impacts will vary greatly due to regional differences in climate, appliance stocks/saturations, energy costs, and demographic trends. In the present work, we use an end-use energy demand forecasting model to assess the energy, peak demand, and economic impacts of the standards for the ten DOE planning regions of the continental U.S.

We find that the standards will save the nation nearly $25 billion (in 1987 dollars) in cumulative net present benefits to 2015. The savings consist of reductions in electricity generation of 800 TWh and in direct fuel use of almost 2 Quads.

We find that the largest absolute and percentage electricity savings will occur in the South Atlantic and Southwest DOE regions due to both the high saturation of air conditioning and the relatively greater cooling loads found in these climates. Conversely, we observe the lowest percentage electricity savings in New England due

to lower air conditioning saturations and smaller cooling requirements.

Percentage savings for all other fuels are relatively modest and uniform across all regions with the exception of the Northwest region where we predict fuel use will increase slightly. In the Northwest, NAECA has the effect of reducing the attractiveness of electricity as a heating fuel because heat pumps (25% of electric heating appliances) become too expensive relative to expected annual heating requirements. In this situation, fossil fuel furnace sales increase, leading to increasing consumption of other fuels.

The analysis is of special significance to electric utility planners because the end-use model we employ shows how the structure of demand will be affected by the standards. For example, we find that, while overall air conditioning equipment sales will change only slightly, sales will shift away from central air and heat pumps in favor of room air conditioners. For water heating appliances, we find that electric water heating sales will increase at the expense of other types of water heating equipment. These effects are small nationwide, but can be significant in some regions.

The end-use detail of our forecasts also allows us to provide guidance to utilities considering rebate programs to stimulate the purchase of even more efficient appliances. We find that only modest rebates ($50-$100/unit) will be needed to stimulate the purchase of more efficient central air conditioners, but that utilities must distinguish between models that do and do not save electricity peak demands. In order to encourage purchases of more efficient refrigerators, we find that a rebate must offset almost the entire incremental cost of the efficiency improvement.

Research and Policy Studies to Promote Building Energy Efficiency in Southeast Asia

M. D. Levine, H. Akbari, J. F. Busch, J. J. Deringer, Y. J. Huang, and K. H. Olson

The purpose of this project is to assist five ASEAN countries[†] to identify appropriate government policy options for buildings energy conservation, to enhance their policy analysis capabilities, and to implement policy initiatives.

Several on-going assistance programs have continued through this past year. First, workshops in building energy audit procedures have been given in ASEAN for several years by LBL consultants. Second, assistance has been provided to several countries in developing energy conservation standards for new commercial buildings. Malaysia is in the process of adopting a new building standard for implementation. Thailand is also evaluating a similar standard that will be voluntary.

A policy options paper has been prepared to define a wide range of policy approaches that could be pursued in addition to building energy standards to reduce energy use in buildings.

The most important new activity of the project has been the development and implementation of research activities on building energy conservation in each of the ASEAN countries. These research efforts are summarized in the accompanying Table. These research activities, as they progress in each of the countries, will yield a deeper understanding of energy use in ASEAN buildings. This in turn will provide a sound technical basis for effective policies to reduce energy use in buildings.

[†]The countries are Indonesia, Malaysia, the Philippines, Singapore, and Thailand.

Table. ASEAN in-country research projects

Country	*Project Title*	*Description*
Indonesia	Policy	Review existing building regulations; conduct building audits; develop energy conservation policy for buildings.
Indonesia	Survey of Energy Use In Hotels and Simulation Studies	Audits of hotels and other commercial buildings; energy analysis using computer simulation tools (DOE-2 and ASEAM.2) to determine cost savings.
Indonesia	Weather/Solar Radiation Data	Collect hourly solar and weather data in Bandung and Jakarta; analyze weather data; develop typical weather year and prepare in DOE-2 format.
Indonesia	Control and Monitoring of Commercial Buildings	Review existing buildings with energy management and control systems (EMCS) in place; review economies and energy savings of retrofit measures; upgrade existing EMCS with new controls and monitoring equipment and monitor building energy use.
Malaysia	Utility Policy	Measure building hourly load profiles using UPLAN simulation code; analyze short- and long-term marginal costs for utility; analyze commercial conservation/load management effects on load shapes; conduct financial analysis of costs, tariffs, and marketing strategies; analyze overall implications for future utility policy.
Malaysia	Chiller Optimization and Control	On-site study of buildings with building automation systems (EMCS) in place; simulate performance of these buildings; compare simulation results with actual.
Malaysia	Energy Audit Studies and Development of Energy Conservation Requirements for Malaysian Buildings	Analyze results of audit survey of 10-12 buildings using ASEAM.2; analyze and revise OTTV equation using solar radiation data; perform DOE-2 studies; assess economics of implementation of standards on existing buildings.
Malaysia	External Shading of Windows	Survey and tabulate use of external shading devices on existing buildings; build physical model to analyze effectiveness of shading devices; correlate results to those of DOE-2 simulations for selected devices; develop shading schedules for DOE-2.
Malaysia	Administration and Policy Studies	Survey 25+ existing government buildings and analyze results; identify possible targets for energy conservation measures; study effect of implementation of policy on existing government buildings.
Philippines	Lighting and Daylighting	Survey and compile results of actual lighting and daylighting conditions in 20+ buildings, including survey of behavioral response to daylight and artificial light; study daylight geometrics, such as glare and brightness imbalance; develop DOE-2 daylight simulations; set up controlled physical models for monitoring.

Country	Project Title	Description
Philippines	Forced and Natural Ventilation	Survey and compile results of actual air conditions and thermal comfort in 12 buildings; correlate ESPAIR computer simulations with findings of survey; prepare design guidebook for natural ventilation.
Philippines	Air Conditioning Equipment	Survey component cooling equipment in 50+ commercial buildings; study effects of air conditioning efficiency improvements using ASEAM.2, and for selected buildings, DOE-2.
Philippines	Performance of Typical Building Insulating and Reflective Materials	Perform correlation studies to determine heat transfer values of materials in non-air conditioned buildings and potentials for comfort conditioning and energy efficient design; establish U-values for typical building cross-sections of materials and components commonly used in the Philippines but not covered by ASHRAE; build test cell to test materials.
Philippines	Analysis, Assessment, and Policy	Survey building characteristics and energy use and also building managers' attitudes toward energy conservation investment; perform detailed energy audits of 50 buildings; study performance of cogeneration systems and investigate utility pricing policy affecting cogeneration use; perform DOE-2 and ASEAM.2 simulations in support of policy development including development of building energy conservation standards; analyze policy issues.
Singapore	Lighting and Daylighting	Extend existing lighting survey of 200 buildings to include industrial buildings and obtain more detailed data from existing 200.
Singapore	Energy Analysis Using DOE-2	Prepare new weather data for Singapore for use in DOE-2; evaluate OTTV equation and develop simplified expression for estimating energy use; assess and validate simplified energy estimation methodologies using survey data; develop algorithms for revised energy standards.
Singapore	Energy Management	Conduct energy measurements in existing buildings; compare results with simulation studies; evaluate energy conservation options; produce manual on energy management.
Singapore	Assessment, Analysis, and Policy	Verify solar correction factors based on a full year of solar data; study conductance heat gains through glass; verify ETDQ values for classification of construction—light, medium, and heavy. revise OTTV handbook; develop approach to the revised standards.
Thailand	Natural Ventilation	Collect and analyze weather data including solar data for Chiang Mai; Using ESPAIR simulation code, conduct natural ventilation studies; produce design guidebook on natural ventilation; organize dissemination workshop.

Country	Project Title	Description
Thailand	Lighting and Daylighting	Perform daylighting studies with DOE-2; evaluate daylighting availability in Bangkok; investigate various design methodologies; conduct experiment to compare effectiveness of installed daylighting controls in an office environment; organize in-country workshop.
Thailand	Air Conditioning Research	Perform parametric study of air conditioning system performance via simulation; evaluate actual performance of air conditioning equipment.
Thailand	Assessment, Analysis, and Policy	Perform audits and analyze data; formulate policies, develop standards and implementation package.

Global Biodiversity: Habitat Change and Species Extinctions*

W. E. Westman

Current concern about the global loss of species arises in part from the rapid rate of clearing of species-rich tropical forests. We are using satellite remote sensing to quantify rates and patterns of tropical deforestation, and are linking this information to predictions of species endangerment by use of field data and predictive models. Current efforts in a pilot study are focused on two tropical rainforest regions: southern Uganda, and northern Queensland, Australia.

In our work in Uganda,[1] using LANDSAT multispectral scanner (MSS) data, we found a net removal of 29% of the forest area in Mabira Forest Reserve during the period 1972-1988 (see Figure). During the same period, the edge-to-area ratio of the forest increased by 29%, and a maximum of 7% of the forest regrew in cut areas. We could also differentiate heavily-logged from lightly- or moderately-logged areas of forest using the MSS data. By linking this information to field-based studies, we could identify which two of seven primate species in the area were expected to thrive differentially under current patterns of forest disturbance.

In Queensland,[2] we conducted field work on the Atherton Tableland to examine how vascular plant species, and an indicator arthropod species (a giant centipede), respond to forest fragmentation over time. The research included an investigation of differences in attributes of plants growing on newer forest edges vs. forest interiors.

In future work, we plan to examine the impacts of forest clearing in Uganda on a larger regional scale using Advanced Very High Resolution Radiometer satellite data (1 km resolution), and to use predictive models from biological theory to predict regional impacts on the biota.

REFERENCES

1. Westman WE, Strong LL, Wilcox BA. *Tropical deforestation and species endangerment: the role of remote sensing.* Landscape Ecology: in review.
2. Westman WE. *Structural and floristic attributes of recolonizing species in large rainforest gaps, North Queensland.* Vegetatio: in review.

*Collaborators were Laurence Strong, Christine Hlavka (NASA Ames Research Center); Bruce Wilcox (Institute for Sustainable Development); Hank Shugart, John Weishampel (University of Virginia); C.J. Tucker (NASA Goddard Space Flight Center). This work was sponsored by the National Science Foundation and the NASA Earth Sciences Division.

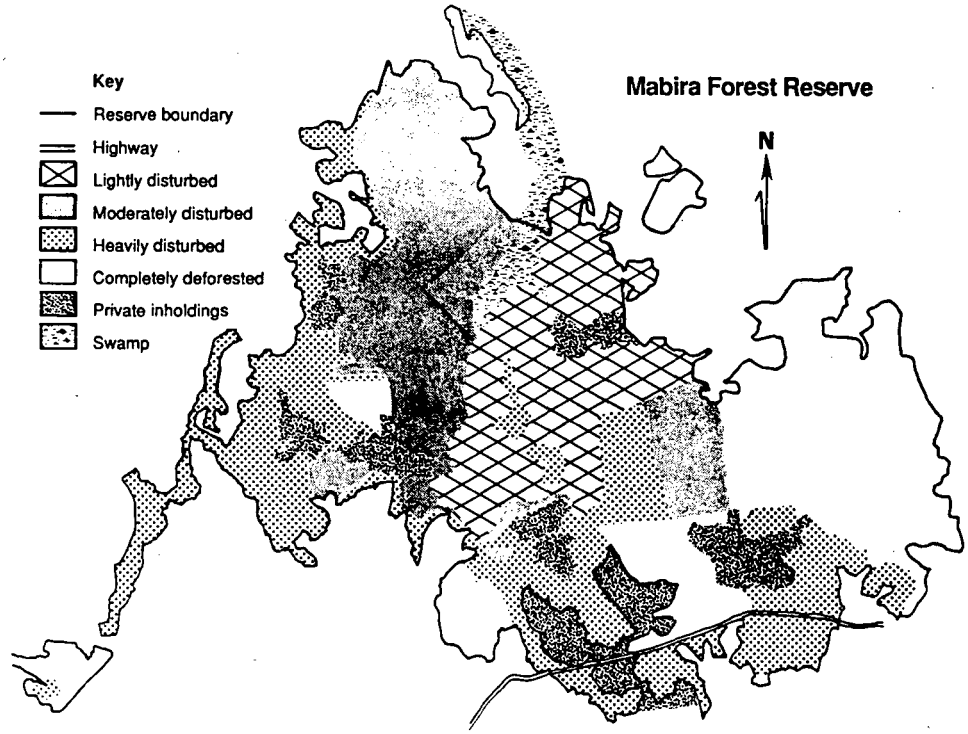


Figure. Mabira Forest reserve in southeastern Uganda, showing disturbance observed during a field survey in 1987-1988. (XBL-8810-3674)

Effects of Climate Change on Vegetation in California and Baja California*

W. E. Westman

General circulation models of global climate predict that California's climate will become warmer and wetter with continued buildup of carbon dioxide over the next century. By observing predicted climate changes for California in relation to existing climatic tolerances of vegetation, we made predictions of vegetation change using direct gradient analysis. We predicted that chaparral elements would expand at the expense of southern oak woodland and blue-oak digger pine woodland; that yellow-pine/mixed conifer and red fir forest elements would expand at the expense of subalpine forests in the Sierra Nevada, and that inland prairie and sage elements would expand into areas now supporting coastal sage and succulent scrub vegetation.

Higher summer temperatures imply an aggravation of ozone formation in coastal southern California. The effects of increased precipitation, increased temperature, and increased ozone levels on the coastal association (Venturan) of coastal sage scrub were examined under varying fire frequency regimes using a simulation model (FINICS).[1] Simulations of the combined effect of these changes (see Figure) indicate that long fire-return intervals (30-40 years) would be needed to maintain mixed-species shrub dominance. This could intensify conflicts between biodiversity goals and current fire hazard reduction practices involving prescribed burning at shorter return intervals.

Some early warning signs of changes in Venturan coastal sage scrub under increased evapotranspirative stress and elevated ozone may be inferred by comparing ecophysiological and morphological changes along a gradient in these parameters in the Santa Monica Mountains. As sites of elevated temperature and ozone are approached, early season leaves of the dominant black sage (*Salvia mellifera*) become larger and less dense, nitrogen and lignin concentrations increase, and the chlorophyll (a/b) ratio decreases. At both coastal and inland sites, reduced shrub cover increases the opportunity for growth of annuals, including exotic grasses.

We plan to expand our simulation modeling to include the behavior of the evergreen shrublands (chaparral) of California, and examine the relative abilities of the evergreen and drought-deciduous shrublands to thrive under future climatic alteration.

*George P. Malanson, Dept. of Geography, Univ. of Iowa, collaborated in this work, which was sponsored by the Environmental Protection Agency.

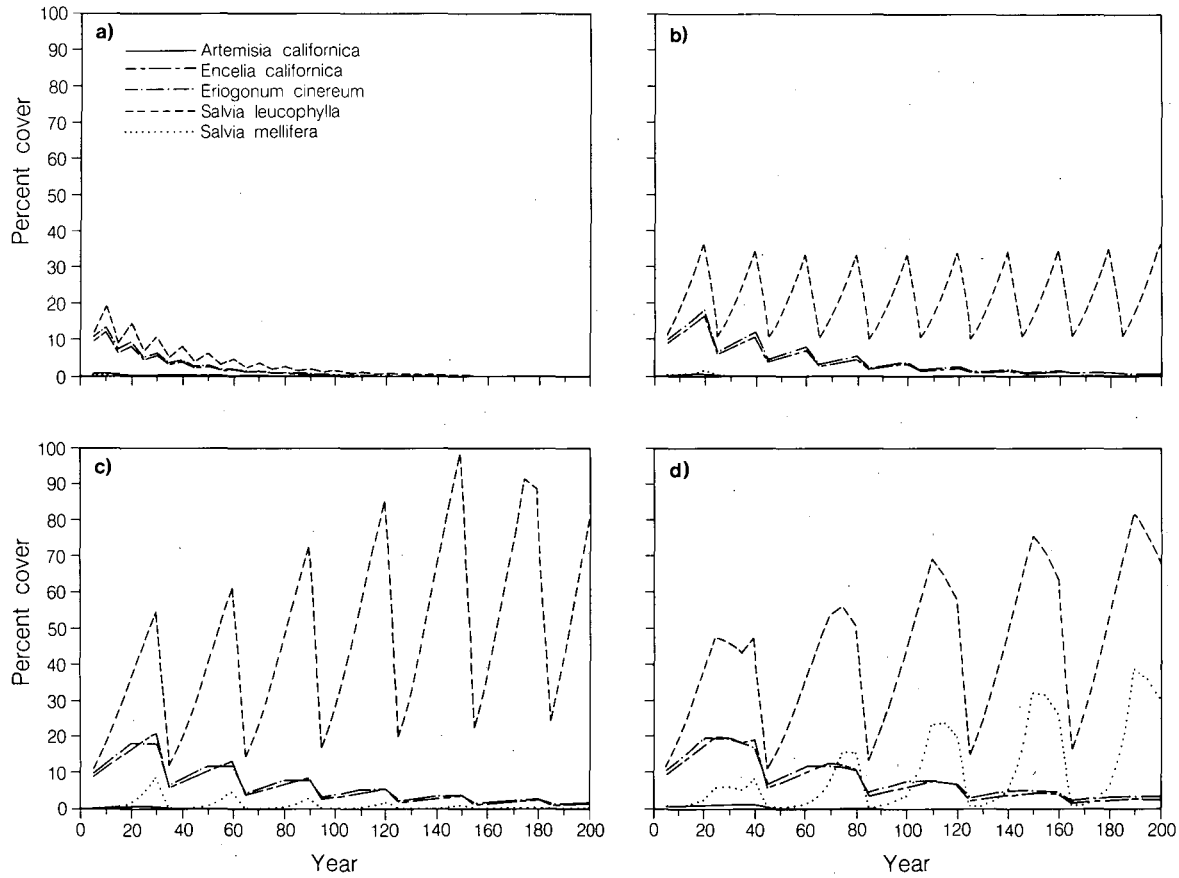


Figure. Changes in percent cover (y-axis) of five species of coastal sage scrub over time (x-axis) under FINICS model simulation, assuming plant growth under the altered climate of doubled carbon dioxide levels, increased ambient ozone, and higher fire intensities. a-d show responses to fire return intervals of 10, 20, 30, and 40 years respectively. (XBL-889-10424)

REFERENCE

1. Westman WE, Malanson GP. "Effects of climate change on mediterranean-type ecosystems in California and Baja California," in: RL Peters, ed. *Consequences of the greenhouse effect for biodiversity*. Yale Univ. Press, New Haven, CT: in press.

Contribution of LDC Energy Use to the Global Climate Problem

J. Sathaye, A. Ketoff, L. Schipper, and S. Lele

Over the last century, the global atmospheric concentration of carbon dioxide and other "greenhouse gases" has increased substantially. This may have serious consequences for human well-being over the next century. Emissions from energy consumption are the single largest contributor to this effect. An examination of possible trends in energy consumption and the potential for its reduction is therefore crucial to any attempt to prevent or delay global warming.

We have explored the contribution of developing countries (LDCs) to the demand side of the problem.[1] We use information about energy and economic activity in the developing and developed countries to construct two basic scenarios for the year 2025 in five regions: Asia, China, Africa, Latin America and the Middle East. These are based on assumptions about economic growth rates, energy price trends, and population growth. We also construct two policy cases to examine the effect policies could have in reducing energy intensity and activity levels in the two basic scenarios. In analyzing energy demand, we examine five sectors in each region: industry, transportation, residential, commercial and agriculture. We establish measures of energy intensity (energy consumption per unit of activity) for each sector, and seek to understand the

changes in structure of that sector that influence its energy intensity. We also examine the changes in the mix of fossil fuels (taken as a group), biomass, and electricity in each sector.

The Table gives the overall results by region for the rapid economic growth scenario. The results for non-LDC regions are derived from basic assumptions consistent with those used for the LDC scenarios. The results show the large shift in share of energy consumption from the industrialized to the developing countries. About half of world energy use takes place in the LDCs in 2025. Modern fuel use increases at 3.4% annually in the LDCs between 1985 and 2025. Almost 80% of the increase in fossil fuel combustion in this scenario occurs in the LDCs. Their contribution to carbon dioxide also increases in similar proportion.

It is estimated that such an increase in energy consumption will lead to a realized temperature increase of 2.5°C by 2050. To place this in perspective, the anticipated temperature rise of 1.5-4.5°C over the next 100 years is equivalent to the temperature increase that has taken place over the last 18,000 years.

We also construct scenarios where strong policies are adopted to control growth in energy use. These would lead to a temperature increase of about 1.5°C by 2050.

REFERENCE

1. Sathaye J, Ketoff A, Schipper L, Lele S. *An end-use approach to development of long-term energy demand scenarios for developing countries*, LBL-25611, Sept. 1988.

European Electric Power Generation: The Role of Oil

D. Hawk and L. Schipper

Annual primary oil demand in European member countries of the Organization for Economic Cooperation and Development (OECD) declined by approximately 25% between 1973 to 1986. Nearly one-third of this decline is the result of the phasing-out of oil for use in electricity generation. In 1973 in France, Germany, Italy, England & Wales, and Sweden, oil was the first- or second-most important energy source for electricity generation—

Table. Energy demand in 1985 and 2025, all regions

	1985	2025 Rapid Scenario		2025 R/Policy Scenario		GDP/Cap.	Pop.
Region	EJ*	EJ	% AAGR**	EJ	% AAGR	% AAGR	% AAGR
C-Planned Asia	29	96	2.9	77	2.4	3.8	1.0
Middle East	9	42	3.7	36	3.3	2.0	2.3
Africa	8	43	3.4	32	2.7	1.7	2.4
Latin America	19	72	3.3	56	2.7	2.8	1.5
S and E Asia	22	85	3.3	66	2.7	3.6	1.5
LDC Total	90	337	3.3	266	2.7	4.5	1.5
World Total	354	642	1.5	514	0.9	2.1	1.3

* 1 EJ is 10^{18} Joules, or about 23.9 MTOE, 0.5 MBDOE, or 0.95 quadrillion BTU.
** % AAGR = % average annual growth rate.
Note: Energy demand includes that for modern and traditional fuels.

generating between 14% to 59% of electricity produced. By 1986, oil use for electricity generation had declined to between 1.5% and 5.6% in all countries except Italy (39.4%), where oil is still being used for base-load generation. However, the oil generation facilities existing in 1973 are still in place and are operable (in various stages of reserve) and some oil-fired generation is used, primarily to meet peak load. Thus, the infrastructure that enables oil-based electricity generation remains in place, but the *intensity* with which oil is used has changed. This sector could trigger a large and quick rise in the demand for oil: a potential 25% increase in the total oil demand for these five countries. The Figure shows the huge increases in oil use by the power sector that would result if the oil-using capacity in each of these countries was used at its highest feasible level (capacity factors between 60% and 79%). The case 1 potential is calculated using only oil capacity. The case 2 potential is calculated using all of the oil-using capacity, which includes capacity with multi-fuel capability.

In England & Wales and Sweden, oil-based generation may soon increase above 1986 levels. In Sweden, oil-based generation will be used to bridge a supply gap that will result from the de-commissioning of nuclear power plants in the absence of new generation capacity to replace it. In England & Wales, a competitive environment introduced through privatization, the relative youth of the oil capacity, and the current low oil prices may cause oil-based electricity generation to have a competitive advantage, even replacing some coal-fired generation. Continued delays in the nuclear program would encourage the use of oil to bridge supply gaps until the nuclear capacity comes on-line or a different generation source is selected. In Italy and Germany, oil-fired electricity generation will likely remain relatively constant. Unless German law changes, no additional oil-based generation will occur. Only in France will oil-based generation decline.

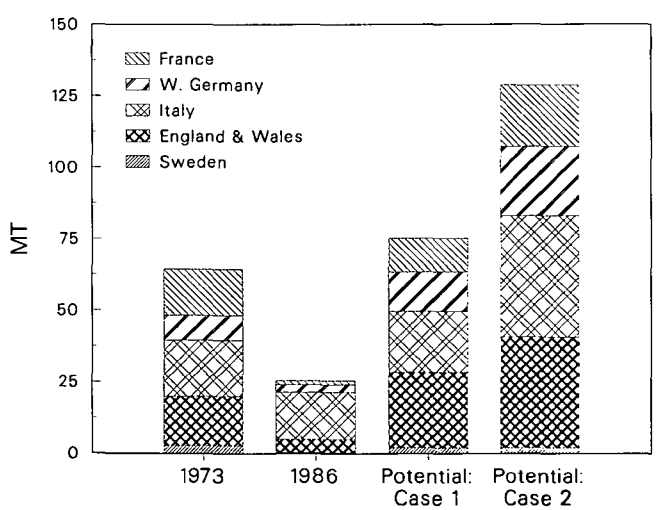


Figure. Oil use by the power sector, past, present, and potential. (XCG 8810-6780)

Although oil-fired electricity generation may increase above 1986 levels in the near future in some countries, the maximum potential levels of oil-based generation calculated in this report will not be attained in any of the countries *unless* a major electricity generation resource or technology suffers a severe, unforeseen disruption. In the absence of such a disruption, institutional barriers against dependence on oil will preclude the realization of the existing potential. Nonetheless, the "hidden" potential for oil use in the power sector, represented by the existing oil-fired capacity, must be borne in mind. As institutions and political agendas evolve, so too might attitudes regarding oil use.

REFERENCE

1. Hawk DV, Schipper L. *The role of oil in electricity generation in five european countries: past, present, and potential*, LBL-25674, draft report.

Residential Energy Conservation Policy and Programs in Six OECD Countries

D. Wilson, L. J. Schipper, S. Tyler, and S. Bartlett

In response to the impacts of high international oil prices in the 1970s and early 1980s, the governments of many countries implemented policies and programs for the purpose of reducing household energy consumption. Through these policies and programs, governments sought to improve the residential energy market (by removing perceived market barriers), change that market (by offering subsidies, charging taxes, etc.), and alter the make-up of items on the market (appliances, heating equipment, etc.). The tools they used to meet these goals were information, subsidies, regulations, and price manipulation.

The current low price of oil has offered governments a reprieve: time to pause and look back. That process is currently taking place within several governments as they anticipate the necessity of moving forward with new programs motivated by changes in energy prices and/or other concerns such as the negative environmental impacts of energy supply and consumption processes. In this study, we describe and compare policies and programs that were implemented in Denmark, France, Japan, Sweden, West Germany, and the U.S. We present them along with contextual factors which determine both policy and program goals and the range of feasible measures/methods for achieving them. Contextual factors include: energy supply and demand structure; political and social environment; economic environment; institutional structures of relevant government agencies; and physical environment (climate, age and thermal quality of the housing stock, etc). Each

of the above-mentioned topics is then discussed individually, using the specific experiences of the study countries to highlight and illustrate our observations with regard to their use.

These analyses have resulted in several fundamental conclusions regarding residential energy conservation program design. The first of these is that the most far-reaching programs take an integrated approach, using more than one tool to achieve a well-defined policy goal. An important example of this took place in Denmark where a program package of subsidies, home audits, and a home labeling program were used to attempt to improve the thermal quality of the existing housing stock. The specific tool or set of tools to be used in a program should be chosen based on both program objectives and context. The implementation of program tools commonly requires combined efforts of a variety of government institutions. The relationships and interactions between these institutions should be directly addressed as part of every program design, and where possible should be enhanced. In addition, relationships between government and non-government institutions (such as industry and academia) should be nurtured. These relationships can provide important channels to consumers and an infrastructure for supporting program implementation. Wherever possible, existing infrastructures should be used to implement programs. Both the Swedish retrofit subsidy plan that was melded into the existing national home loan program and the program in Germany that supported the publication of energy efficiency information through a well-known and widely-read magazine provide examples of this. A multitude of examples of problematic programs that attempted to create and rely exclusively on new institutions and infrastructures also exist. Finally, program evaluation should be part of every program design. Evaluations should be used both as part of the implementation process (i.e., learning and adapting as you go along) and after programs are completed (i.e., enhancing the learning curve effect). Although program evaluations have become more common in the U.S., they are still relatively sparse in other countries (except Sweden). Removing the many barriers to program evaluations should be a high priority goal of policy- and decision-makers responsible for initiating and/or planning residential energy conservation programs.

Home Electricity Use in OECD Countries: Recent Changes

L. Schipper, D. Hawk, A. Ketoff, and N. Hirt

The Home Electricity Use Study* has been recently updated to study changes through 1987.[1] These changes suggest that the wave of increased efficiency seen in our earlier study has peaked. Except for the heating market, inter-country differences are shrinking. The inter-country comparison suggests that many factors besides price and income influence the levels and patterns of residential electricity use in homes of the Organization for Economic Cooperation and Development (OECD) countries.

The Figure shows per-capita use in 1986 divided into end uses. The most important difference among countries is the use of electric space heating, a dominant component of sales growth in France, Sweden, and Norway. Secondary use of electricity for heating, i.e., in combination with other main heating systems, has grown in Denmark and is now a leading component of growth in electricity in Japan, where heat pumps reach the 50% saturation level.

The historical evolution of the countries shown in the Figure reveals that once homes reach a level of consumption corresponding to about 1000kWh/cap. for lighting, appliances, and cooking, then household electricity use only grows significantly if electricity makes significant inroads against fossil fuels in the space and water heating markets. In Sweden and Norway, such gains drove strong increases in household electricity use in the late 1970s and 1980s. In these countries, electricity heats 35% and 65% of all homes, respectively. In the Netherlands, by contrast, electricity heats almost no homes: instead cheap gas provides space heat, hot water, and cooking for over 90% of homes.

Differences in structural features, such as housing and appliance characteristics, incomes, and habits and lifestyles are not insignificant but many of these differences have diminished over time. This is particularly true for electric appliances. As the number of major international appliance manufacturers has declined, appliances have become more homogeneous.

If the differences in use patterns shown in the Figure are analyzed further, significant differences in intensity, or use per household, are found. For example, homes with electric water heating in Germany use considerably less

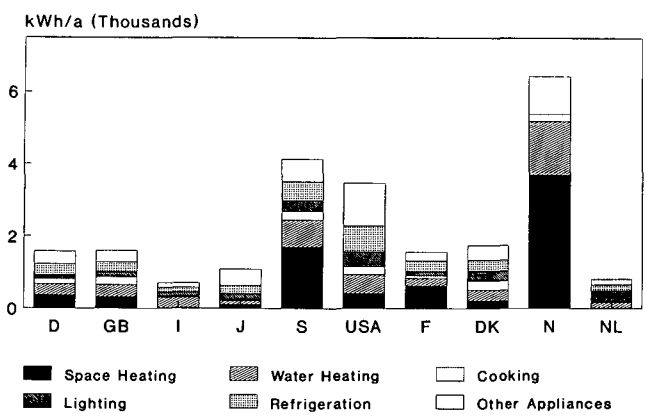


Figure. Electricity use per capita in 1986, climate corrected. D = West Germany, GB = Great Britain, I = Italy, J = Japan, S = Sweden, F = France, DK = Denmark, N = Norway, and NL = Netherlands (XBL-8811-3856)

*This work was additionally supported by the International Energy Agency, Paris, France and Oslo City Light, Oslo, Norway.

electricity per home for that purpose than those in the U.S., Sweden, or Japan. German homes use instant water heaters with almost no tank losses, while Japanese, American, and Swedish homes use large tanks.

The efficiency of electric appliances has increased markedly in most of the study countries. These improvements limited the growth in appliance electricity use caused by increased saturation levels; in a few countries (Denmark, Sweden, United States), growth in use per household was very slow or even negative after 1978. Appliances sold in 1988, while far more efficient than similar ones sold in the early 1970s, may not be significantly more efficient than those sold in 1985. If this "efficiency plateau" proves lasting, then electricity use for appliances could begin to grow again as larger and more fancy models appear in households. Our comparisons also suggest that there are slight differences in the sizes and efficiencies of appliances within European countries; in countries with high electricity prices, such as Denmark and Germany, efficiency is slightly higher than in countries with lower prices. Appliances in North America are larger and less efficient than their European counterparts.

The price of electricity is an important determinant of the level of demand in the long run. If cheap compared to fossil fuels, electric heating gains a high market share (as in Norway), and water heating becomes attractive as well. Prices also influence comfort and lighting levels, and have some impact on appliance size and use. Income is an important determinant of the level of demand while stocks of major appliances are growing, but becomes less important thereafter, particularly in countries where the most expensive appliances are often the most electricity-efficient ones. Technology—the choice of heating system and insulation and the actual design of appliances—is certainly influenced by electricity prices, but other factors, such as climate, the presence of central space- and water-heating, and the traditions of the housing industry also influence the design and use of appliances.

Work in FY 1989 will focus on four areas. First, we shall continue our dialogue with the major appliance manufacturers to better quantify the savings in electricity use since 1973 that have arisen from greater efficiency. We will also explore the factors driving the future appliance market, and how new appliance features will influence electricity consumption. We will extend the comparison of household electricity use to 1987, with special emphasis on a Scandinavian comparison. Thirdly, we will explore the impact of certain kinds of lifestyle changes on future electricity use. Finally, we will extend our analyses to cover important end uses in developing countries, based on direct experience with surveys in Venezuela and Indonesia as well as information generated from our urban energy-use network.

REFERENCE

1. Schipper L, Ketoff A, Meyers S, Hawk D. Residential electricity consumption in industrialized countries: changes since 1973. *Energy* 1987; 12:12:1197-1208.

Electricity in the LDCs: Trends in Supply and Use Since 1970

S. Meyers and J. Sathaye

The share of world electricity production accounted for by the less developed countries (LDCs) grew from 11% in 1970 to 20% in 1986. The average annual growth rate for LDC electricity production in this period—8.4%—was over twice the rate of 3.8% in the "developed" countries. Growth in the 1980s—6.7%/year through 1986—has been less than the rate of 9.4%/year in the 1970s, mainly due to slower economic growth in Latin America and Africa.

Electricity production has grown fastest in Asia (9.5%/year between 1970 and 1986), followed by China (8.8%/year), Latin America (7.7%/year), and Africa (6.4%/year). Among the 13 countries in our study, growth ranged from 5.2%/year in Argentina to 13.2%/year in South Korea. Indonesia, Malaysia, and Thailand averaged growth in excess of 10%/year, and Pakistan, Taiwan, and Brazil were close to this.

Electricity generation is much higher in China (450 TWh in 1986) than in any other LDC. Brazil (212 TWh) and India (202 TWh) are also major producers of electricity. The next largest—Mexico, South Korea, and Taiwan—are well below India.

The share of total LDC electricity production derived from fossil fuels has remained at about 65% since 1970. The share of fossil fuels in 1986 was 77% in China and Africa (56% if South Africa is excluded), and 70% in Asia. In Latin America, the hydropower share increased from 51% to 61% between 1970 and 1986. Hydro's role has increased in China since 1970, but has declined in Asia and Africa.

The LDCs have experienced a shift away from oil to coal, natural gas, and nuclear power (mainly in Asia). Coal dominates power generation in China and India, and is also prominent in South Korea and Taiwan. Natural gas plays an important role in Pakistan, Thailand, and Venezuela. For 12 major LDCs, the combined share of oil in total public generation declined from 27% in 1970 to 17% in 1986. The share of hydro fell from 48% to 44%, coal grew from 15% to 22%, while nuclear went from 2% to 9%.

The extent to which electricity consumption grows faster than the economy depends in part on the stage of economic development in which a country finds itself. The ratios between average growth in electricity consumption and growth in real GDP in the 1970-86 period in the 13 study LDCs were mostly between 1.6 and 1.9. The ratio was lower in Taiwan and Malaysia, reflecting their more mature level of economic development.

The industrial sector dominates electricity consumption in nearly all LDCs, but its share of total consumption has generally declined in the face of faster growth in the residential and commercial sectors (see Figure). Residential electricity use per capita has grown at more than 10%/year in most of the countries due to increase in the

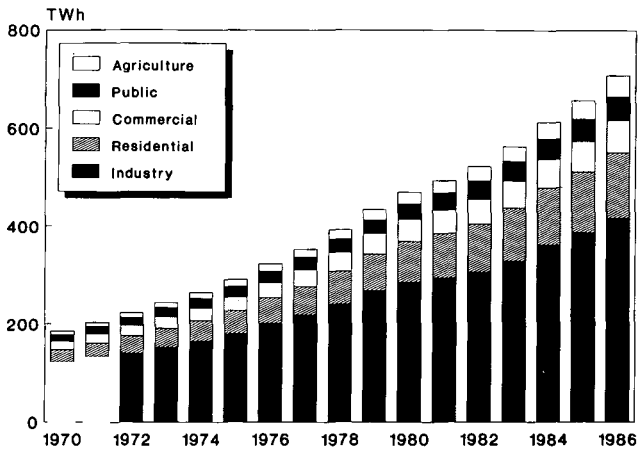


Figure. Electricity consumption by sector for 12 LDCs. (XBL-8810-3591)

number of homes that have electricity and rising ownership of appliances.

As electricity demand grows, many LDCs face increasing difficulty as they seek to expand supply and maintain existing systems. Power shortages are critical in many countries and environmental issues are becoming more important. Measures that are receiving closer attention include reform of tariffs to better reflect costs, reducing demand through end-use efficiency improvement, encouraging private power generation, and improving technical and managerial aspects of electric utilities.

REFERENCE

1. Meyers S, Sathaye J. *Electricity in the LDCs: trends in supply and use since 1970*, LBL-26166, 1988.

Production, Consumption, and Trade of Natural Gas: Western Europe and the Developing Countries

J. Sathaye, A. Ketoff, and G. Pireddu

World-wide, natural gas is assuming growing importance. It is being discovered in increasing quantities in the developing countries and it is also the fuel of choice to substitute for oil in oil-importing countries. It is environmentally more benign than other fuels and emits less "greenhouse gases" relative to those associated with the use of oil and coal. For these reasons, its use will be highly valued in the future.

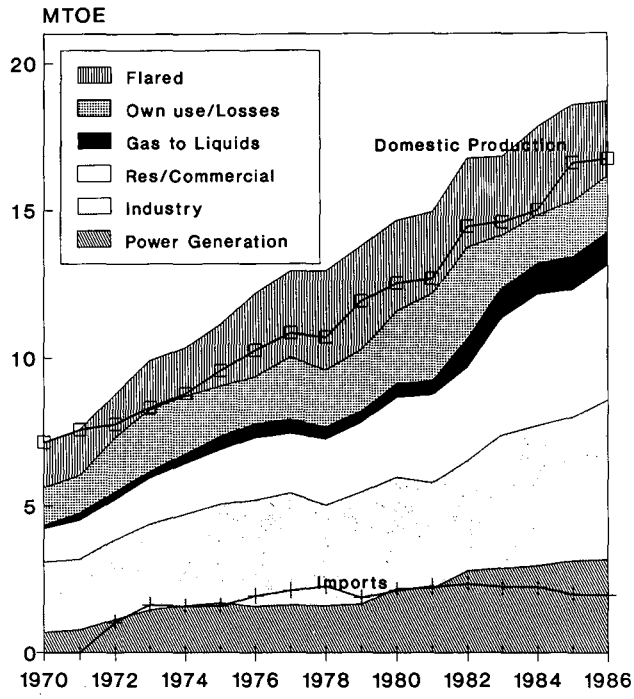
This work is intended to describe the current and potential use of natural gas in several regions of the world—Western Europe, Asia, Latin America, and the Middle East. Within each region, we focus on a few countries that are in a position to export, or are already exporting, natural gas to other countries.

In Western Europe, natural gas demand is not expected to increase by more than 10-20% by the end of the century. The major uncertainty is whether the Scandinavian countries will use more of the abundant gas available in that region for power generation and space heating. The long-term demand for gas could increase considerably if environmental policies forced additional displacement of other fuels.

The Asian region (not including the Soviet Union) accounts for about 6% of the world's natural gas reserves. Indonesia, Malaysia, Brunei, and Afghanistan have deposits large enough with respect to domestic demand to export natural gas. Taiwan and Japan have smaller and dwindling deposits of natural gas. The region is far from fully explored and new discoveries have been reported in Papua New Guinea and India. Asian reserves are expected to increase over the next two decades. Natural gas utilization will depend on the location of the natural gas deposits within a country and the level of reserves relative to the country's needs. Countries that discovered natural gas recently have used it in industry and power generation. Residential use occurred in countries that had heating needs and those that discovered gas some decades ago. Exports of gas, either as LNG or methanol, from Malaysia and Indonesia will remain a long term option; those from other Asian countries are unlikely given their current reserves and indigenous demand for natural gas.

Natural gas in Latin America has changed from being a by-product of the petroleum industry in the 1960s and the early 1970s to become an important energy source for the indigenous market. The prospect for export of natural gas from this region is limited. Demand is growing in the three major producing countries—Argentina (Figure), Mexico, and Venezuela—and is likely to expand in the others, particularly in Brazil. Increasing demand can be expected in the residential sector as a result of both an increase in the number of users (in Venezuela and Mexico) and an increase in comfort levels (in Argentina). Use in transport will remain minimal, although it might grow considerably in certain markets if strong government programs are launched. Industrial demand will remain dominant, particularly as the use of gas is seen as beneficial either to the environment (e.g., in Mexico), or to the international competitiveness of local industry (e.g., in Venezuela). With both Venezuela and Mexico pushing the use of gas as raw material for petrochemicals, demand in this sector is bound to increase considerably. Both countries would rather export higher-valued petrochemicals than LNG. Given present trends in demand patterns in Latin America, reserves of natural gas appear insufficient to allow export in the long run. Furthermore, since most of the gas is associated with oil, gas for export would be available only when demand for oil, and therefore production of oil, is high.

The cost of natural gas in the Middle East is minimal, since its production is associated with oil. Final users are



Source: IES/LBL.
Own use/Losses includes gas reinjected.

Figure. Natural gas in Argentina. (XBL-8812-4249)

charged low prices to favor its use over other, more exportable, petroleum products. Gas demand (in producing countries) will continue to expand as petrochemicals, power generation, and large industries switch off oil products. The uncertainty of the international oil market will push governments (in particular, Saudi Arabia and Kuwait) to seek non-associated resources to be tapped in case of shortages of associated gas. Capital availability might be a constraint, but the priority is high as countries prefer to keep oil underground in a period of low oil prices. In Iran, additional marketable production requires considerable amounts of capital, as major fields are scattered in the southern regions of the country. The end of the Iran-Iraq war is likely to boost industrial demand as well as residential use in newly reconstructed cities, which might justify increased efforts on the production side. As local use of gas becomes a key element of economic development, exports are not likely to be sought by any of the countries examined, with the exception of Qatar and Abu Dhabi. In the other countries, we can expect natural gas to be used in petrochemicals, fertilizers, and other energy-intensive products which will be marketed locally and/or exported.

With increasing discoveries of natural gas world-wide, the likelihood of additional gas becoming available for export in the form of LNG or, after transformation, in the form of methanol is strong.

Energy Markets and Energy Demand: China and the U.S.

J. Sathaye, L. Schipper, and M. D. Levine

Knowledge abroad about China's energy demand patterns and its likely future growth of demand is limited. Likewise, Chinese planners are eager to seek additional information and knowledge about energy use and government policy in the U.S. In order to exchange information and viewpoints, a symposium was sponsored jointly by the State Planning Commission of China and the Office of Policy, Planning and Analysis of the U.S. Department of Energy. The Chinese-American Symposium on Energy Markets and the Future of Energy Demand was organized by the Energy Research Institute of the State Economic Commission of China, and Lawrence Berkeley Laboratory and Johns Hopkins University from the United States. It was held in Nanjing, China in late June 1988. It was attended by about 15 Chinese and an equal number of U.S. experts on various topics related to energy demand and supply.

The Chinese papers provide an excellent overview of the emerging energy demand and supply situation in China and the obstacles the Chinese planners face in managing the expected large increase in demand for energy. Topics discussed by speakers included energy demand modelling, energy pricing reform, air pollution and energy use, and patterns of energy use and conservation in buildings, transportation, industry, and power generation.

The huge rate of economic growth in China has brought with it a dramatic increase in energy use. Energy conservation, however, has not yet surfaced as a common concern or practice among the populace, and lack of price incentive for conserving energy has allowed a huge incremental increase in energy use to accompany China's approximately 10% annual rise in GNP. Of great concern to China's leaders is that country's energy pricing structure, which encourages inefficiency and discourages conservation. "Planned" (i.e., subsidized) prices are replaced in practice by locally derived prices, which in turn often yield to black-market prices. Representatives of the Chinese government expressed their eagerness to reform pricing and to develop and implement conservation techniques and policies.

Conference participants also discussed China's efforts to control indoor and outdoor pollution, especially in urban areas. In China, almost all cooking is done using low-quality coal that is not cleaned (cleaning reduces substantially the sulphur content of the coal). In addition, scrubbers are not yet used by coal-fired power plants. Acid rain has resulted from these practices, and damage caused by acidic pollution is glaringly evident: a slide presentation at the conference depicted two sides of a monument, its windward side pitted and its leeward side, smooth.

Future work with the Chinese is likely to involve collaborations on such topics as energy pricing reform, energy demand and global warming, and building energy conservation. A follow-on conference in which the Chinese researchers travel to LBL is envisioned in FY 1991.

Competition in Electricity Generation

E. Kahn

Competition in the generation of electricity began with the Public Utilities Regulatory Policy Act (PURPA) of 1978. PURPA required regulated utilities to purchase the output of certain private, unregulated suppliers at prices based on the cost of equivalent power. Producers who met the technology specifications embodied in PURPA, essentially cogenerators and users of renewable energy, were called Qualifying Facilities (QFs). The response to PURPA was very substantial in regions which offered favorable terms. In some cases, the response overwhelmed utilities and their regulators, creating a need to ration or limit QF supplies. This unanticipated development spurred interest in reforming the PURPA process to make it more efficient. The principal reform which has emerged from these concerns is the creation of auction or bidding systems in which PURPA suppliers compete for the right to sell under long-term contracts. PURPA auctions raise many design and implementation questions. These have been studied in detail previously.

The Federal Energy Regulatory Commission (FERC) has taken the initiative to broaden the PURPA auction process initiated in individual states. In a series of Proposed Rules, the FERC has suggested expanding the scope of competitive bidding to include all sources of supply instead of only the QFs. The principal effect of the proposed FERC rules would be to create a new class of unregulated suppliers, called Independent Power Producers (IPPs) who would compete with the QFs and regulated producers for the right to provide new generating capacity. The far-ranging nature of the FERC proposals raises a number of policy and technical questions.

We examined the welfare impacts of the FERC proposals in light of prospects for regulatory policy. PURPA and the FERC initiatives have arisen in part out of dissatisfaction with the performance of regulation, particularly with regard to inducing efficient investment in generation facilities. Three scenarios for future regulatory policy were delineated and used as a background against which to evaluate the FERC proposals. These scenarios are: 1) capital minimization, in which utilities avoid investment due to hostile regulation, 2) joint responsibility, in which regulators share planning authority explicitly with utilities, and 3) optimal risk aversion, in which utilities avoid risky investment, but there is no sharing of responsibility with regulators. The balance of costs and benefits varies in each scenario. Depending on the degree of competition between the IPPs and regulated suppliers, there will be no differences in bargaining power and flexibility. Efficiency gains will be obtained, but at the price of higher transaction costs. On balance, the FERC proposals appear beneficial. Details are available.[1]

The FERC proposals imply major changes in the structural organization of the electric utility industry. The underlying assumption that the wholesale generation market is workably competitive implies that the traditionally vertically-integrated and regulated firm will be altered significantly. The key element in these long-run changes is the evolution of the transmission system. The FERC proposals do not explicitly take up the questions raised about transmission under wholesale competition. Any system which evolves must provide for system security, efficient pricing of transmission services in the short-run, and capacity expansion in the long run. Achieving all three objectives will require some kind of cooperative arrangement between the buyers, who will probably end up operating the system, and the sellers, who may have to bear the financial burden of expanding capacity to reach new markets.

The planning and operating environment will also change substantially under wholesale competition. Contractual arrangements will play a larger role in unit commitment and economic dispatch. The utility's obligation to serve will be tested as its "supplier of last resort" function gets defined more precisely. It is plausible that the overall level of wholesale generation reliability may degrade somewhat. Storage technologies, which provide an inventory function, will play a larger role in smoothing out these problems.

There can be expected to be major re-allocations of assets among firms. Some of this will involve divestitures that move particular resources to higher valued uses. More important will be consolidations that will help to make the market operations more efficient. On the buyers' side, small distribution companies can achieve important efficiencies through merger. One problem is that many of these companies are publically owned, and lack the financial incentives to consolidate. Mergers among suppliers will not be harmful as long as monopoly power does not accumulate. The prospects are good that these abuses can be prevented. Detailed results are available.[2]

Future work on these issues will focus on implementation problems of designing all source competitions for bulk power and the resource planning problems these must address.

REFERENCES

1. Kahn E. *Welfare and efficiency benefits of all sources bidding*, LBL-26212, 1988.
2. Kahn E. *Structural evolution of the electric utility industry*, LBL-26165, 1988.

BUILDING ENERGY SYSTEMS PROGRAM STAFF

Michael A. Wahlig, Program Leader

Brandt Andersson
Bruce Birdsall
Fred Buhl
William Carroll
Dominique Dumortier
Kathleen Ellington
Ahmet Erdem
Brenda Hatfield
Robert Hitchcock
Ronald Kammerud*
Jean-Michel Nataf
Cindy Polansky
Joseph Rasson†
Edward Sowell‡
Charlotte Standish
Mashuri Warren
Frederick Winkelmann*

*Group Leader
†Engineering Division
‡Participating guest

BUILDING ENERGY SYSTEMS PROGRAM

INTRODUCTION

The main theme of the Program is the comprehensive simulation, analysis, monitoring, and evaluation of the energy performance of whole buildings, emphasizing nonresidential buildings. Many of the projects develop and apply comprehensive computer models that enable integrated performance analyses of heating, cooling, and daylighting systems. A further activity involved research on absorption heat pumps for solar cooling and gas-driven applications.

The Simulation Research Group maintains and continues development of DOE-2, a public-domain computer program for detailed, hour-by-hour simulation of energy use in buildings. DOE-2 is in wide use in the U.S. and thirty other countries to design energy-efficient buildings and to research innovative building technologies. During FY 1988, new capabilities were added to DOE-2, enhancing its usefulness.

The Simulation Research Group is also developing the next generation of simulation software, for use in the 1990's and beyond. A plan has been formulated in collaboration with groups in the United States and United Kingdom to create an "Energy Kernel System" consisting of an extensive library of software modules and an executive program that will allow users to produce a wide variety of customized simulation programs. In FY 1988, LBL continued development of the Simulation Problem Analysis Kernel (SPANK) as the first prototype of the Energy Kernel System.

The Building Systems Analysis Group continued investigating the performance impacts of energy technologies in nonresidential buildings. As part of a bilateral research agreement, a simplified technique for evaluating long-term energy performance of daylit buildings (based on short-term monitored data) was applied to buildings in the United Kingdom. The technique has proven to be useful, and its continued application and refinement—focusing on energy performance of atria spaces—are being undertaken as part of U.S. contributions to an International Energy Agency (IEA) collaboration.

In collaboration with the IEA Task XI work on passive commercial buildings, we have begun to investigate the daylighting, heating, cooling, and functional effects of atria in large buildings, including the resulting comfort conditions. We have developed new simulation tools to evaluate atrium effects.

A project was initiated to develop a methodology for sizing thermal energy storage (TES), used in cooling systems of nonresidential buildings. Simulations were carried out for two prototypical buildings in three diverse climates in order to identify the climate, design, and operating variables that are significant in determining cool-storage-capacity requirements (and that therefore must be accounted for in the sizing methodology). Existing calculation techniques were found to be acceptable for use in TES sizing from a mathematical perspective, but accepted applications practice must be modified in order to avoid undersizing the system (with resultant loss of cooling).

Development of a computerized tool for evaluation of the energy consumption impacts of retrofit measures in institutional buildings was initiated. This project was motivated by an evaluation of the DOE Institutional Conservation Program completed during the previous year. The evaluation indicated that estimates of energy savings due to retrofits based on monitored data are often at least partially masked by changes in energy use caused by retrofit-independent alterations in the functional or operational environment of the building. The tool being developed allows estimates of energy savings to be corrected for these additional changes, thereby improving the quality of retrofit evaluations.

Several small projects—new-building and retrofit studies—have been carried out for the U.S. Army Corps of Engineers, Construction Engineering Research Laboratory, examining the energy performance of Department of Defense (DOD) facilities. Most notably, simulations compared the energy performance effectiveness of existing DOD building design standards with new federal standards developed by the Department of Energy. For most of the building and climate combinations examined, the existing standards proved to be at least as stringent as those now being promulgated.

The Absorption Heat Pump Project continued research on regenerative absorption heat pumps for high-efficiency solar-driven and gas-driven systems for cooling and heating. As part of a joint U.S./Israel effort, computer models are being developed to enable the detailed analysis and design of these and other new types of advanced absorption heat pumps. These models were used during FY 1988 to simulate the performance of three specific types of high-efficiency absorption cycles, for a wide range of configurations and operating conditions. In addition, an initial cost estimate was made for one of the heat pumps.

Building Systems Analysis*

R.C. Kammerud, B. Andersson, B. Birdsall, W.L. Carroll, D. Dumortier, B. Hatfield, R.J. Hitchcock, J. Eto, F. Winkelmann, and E. Vine

ATRIUM RESEARCH RELATED TO INTERNATIONAL AGREEMENTS

In FY 1987, LBL developed a strong collaborative arrangement as part of the US/UK Bilateral Agreement to use a monitored British building to test a daylighting evaluation method. Because the United States is doing far less monitoring of commercial buildings than are several European countries, this relationship with LBL atrium research is being continued and extended to the broader-based International Energy Agency Task XI on Solar Commercial Buildings.

The United States committed LBL to a limited role in IEA Task XI, as Leader of Subtask B (Simulation) and active member of the Task's Atrium Working Group. LBL is also continuing to work with the UK, both within the Bilateral Agreement and as part of the IEA Atrium Group.

The atrium work completed in FY 1988 focused on developing tools that can be used to better evaluate the critical issues in atria, namely the interplay of daylighting and thermal-energy conservation techniques, as well as the resultant comfort levels in the atrium. Several buildings were evaluated for possible inclusion in the LBL atrium simulation plans.

As Subtask Leader, LBL provided considerable assistance to the IEA Task by coordinating simulations and by providing weather data, software, and expertise to members of the Atrium Working Group and other participants in the Task. LBL has also acted as a conduit for significant information exchange between U.S. and European researchers.

Two key buildings were selected for detailed atrium simulations, one in Norway and the other in the UK. Data on the construction and monitoring of these buildings will be provided to LBL as a basis for the simulation studies. Three additional buildings were identified for further testing of the daylighting evaluation method, two in the UK and one in Sweden.

Initial building simulation models will be established for each of the atrium buildings. The results from these simulations will be compared to data provided from the building monitoring, and modifications will be made to the input descriptions until the model provides an accurate representation of the actual building results. Site visits will be made to both buildings in March in order to clear up any remaining discrepancies.

Figure 1. Gateway 2 Office Block, Oxford: UK/US Atrium Case Study. (XBB 8812-11756)

Simulations will test the sensitivity of atrium energy use to glazing modifications, ventilation, daylighting effects, HVAC integration options, and controls and building operation. Resulting comfort conditions in the atria will be evaluated to determine the potential functionality of atria under different energy scenarios.

LBL will act as consultant and provide support as needed to the British and Swedish researchers applying the daylighting evaluation method (DPEM) to their buildings.

THERMAL ENERGY STORAGE SYSTEM SIZING

The use of cool storage to provide air conditioning in commercial buildings is becoming a widely accepted load management technique. Electric utilities are providing favorable off-peak rates to encourage shifting the air conditioning load away from peak periods. Utilities benefit by deferring addition of new generation capacity and by making better use of efficient base load plants; the customers benefit by having lower electricity bills.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of State and Local Assistance Programs, Institutional Conservation Program Division, the Office of Solar Heat Technologies, Solar Buildings Technology Division, and the Office of Buildings and Community Systems, Building Systems Division of the U.S. Department of Energy; and by the Electric Power Research Institute and the United States Army Construction Engineering Research Laboratory through the Department of Energy, under Contract No. DE-AC03-76SF00098.

Although some storage systems have been undersized, most are believed to have been oversized, detracting from their economic effectiveness. This is difficult to confirm or refute because the existing literature on sizing procedures and performance does not allow the effectiveness of installed systems to be assessed as it relates to sizing. Our project was undertaken to 1) identify the major problems with sizing cool storage systems, 2) develop a preliminary sizing methodology, and 3) identify long-term research issues relating to thermal energy storage in buildings, and 4) develop a plan for addressing these issues.

Sizing methods used for conventional cooling systems are not directly applicable to thermal energy storage systems which operate on a diurnal (or possibly longer) cycle. For conventional cooling systems, equipment size is determined by the peak rate of extraction of thermal energy from the air stream at the cooling coil, accounting for coincident supply air requirements for all zones in the building. In contrast, sizing of cooling systems using thermal energy storage must be based on estimates of peak extraction requirements for all zones integrated over the operating cycle; design sizing must be based on the hour-by-hour coil load profile.

In our study, these coil load profiles were calculated for prototypical buildings using DOE-2. Simulations examined hourly and daily cooling capacity requirements during the cooling season for a 20,000-square-foot, single-story office building and for a 160,000-square-foot, two-story building serving only retail sales functions. The buildings were simulated for Miami (Florida), Dallas/Fort Worth (Texas), and Chicago (Illinois) climates using TMY weather data. These building types and climates were selected because they represent relative extremes, effectively bounding the range of storage sizing issues of importance. Analyses did not include simulation of any specific storage system; instead, buildings were simulated with a conventional cooling system; daily coil energy requirements were interpreted as the total capacity that must be available from the cooling system. This energy may be supplied by a combination of storage and chiller (partial storage or demand-limiting strategy) or by the storage system alone (full-storage strategy). Peak daily coil-energy requirements define the necessary storage capacity.

Based on these simulations, we concluded that the peak integrated load occurs during multi-day periods of severe weather. These periods typically do not include the most severe day or hour in a particular climate; for this reason, traditionally accepted descriptions of peak climate characteristics are inadequate.

We found that much of the integrated coil load at peak consists of energy accumulated during periods when the building is not cooled and is allowed to reach space temperatures above the design temperature. Under these conditions, energy is stored in building materials and furnishings that must be removed by the cooling system in order to satisfy comfort requirements during the subsequent occupied period. The magnitude of the stored energy at peak depends on the length of the uncooled period and of the severe climate period, and on a host of building design parameters relating to thermal capacity and climatic interactions. The magnitude of the peak is also substantially influenced by internal gains and climate interactions considered in sizing calculations for conventional systems.

The only sizing calculations believed to account adequately for the full range of variables that affect peak integrated loads are hourly simulations; this is the sizing procedure recommended here. Guidelines have been documented in order to ensure that the simulation provides a technically sound estimate of peak integrated loads on which to base the storage capacity calculation. Of particular importance, these guidelines ensure that the simulation effectively approximates the heat removal characteristics of a storage system. It is believed that this is a major source of error in sizing TES systems.

We have also considered the appropriateness of other sizing calculation techniques, most notably the simplified method currently recommended by ASHRAE and widely used in design of conventional systems. This method, based on cooling-load factors (CLFs) and on cooling-load temperature differences (CLTDs), can provide reliable estimates of peak integrated coil loads if three refinements are made: first, the CLFs and CLTDs must be refined to provide an improved estimate of the underlying coil load under steady periodic climate and operating conditions; second, a method must be developed for superposing that portion of the coil load that is due to deviations in building operating schedule from the steady periodic assumptions. A preliminary suggestion in this regard has been investigated as part of this project; third, a representation of peak climate conditions that reflects multi-day climate severity must be developed. Preliminary suggestions in these regards have been made.

ICP RETROFIT ENERGY SAVINGS ESTIMATION MODEL (RESEM)

To improve the quality of aggregate estimates, Lawrence Berkeley Laboratory is developing a building-specific Retrofit Energy Savings Estimation Model (RESEM) for the DOE Institutional Conservation Program (ICP). RESEM is a user-friendly tool that will allow state and regional ICP staff to use readily available information for reliably determining the energy and cost savings directly caused by ICP-supported retrofits for a single building. |For maximum accuracy and validity, pre- and post-retrofit energy use (and thus savings) must be directly based on utility billing data.| In FY 1988, we developed design and performance criteria for RESEM, developing methodologies that could not be acquired elsewhere, and began software implementation of the tool.

Technical Capabilities and Methods

RESEM is sophisticated enough in its energy modeling to reflect explicitly the influence of a wide range of design, operation, and weather parameters, as well as the full range of actual building designs and specifications actually

encountered in ICP. The model also interacts with the full range of Energy Conservation Measures (ECMs) allowed under the ICP program.

The engineering model used in RESEM is based on existing public domain methods and algorithms in order to minimize validation efforts and to provide a credible finished model. Building energy consumption is broken down into components of fuel type and end use. This breakdown is key to both the billing-data reconciliation process and the allocation of savings to specific ECMs.

The basic premise of the energy model calibration is that a building's actual utility billing history is the most reliable starting point for determining "real" savings resulting from ECM installation. RESEM uses a specially developed method to accomplish this reconciliation, yielding a "calibrated" modification of the building input description (thereby reproducing actual billed consumption). Reconciliation is done for pre- and post-retrofit building configurations.

RESEM uses a specially developed allocation method for estimating the effects of each ECM in producing the total observed energy savings. To the degree allowed by the energy simulation model, this method takes into account the interactive effects that occur when multiple ECM are installed simultaneously.

Other Features

RESEM is designed to run on currently available, "upper-end" PCs and workstations, decentralizing ECM savings analyses to state and regional levels. RESEM runs fast enough that the session time for an interactive analysis consists mostly of the time the user needs to collect, organize, and input data.

RESEM is a self-contained and complete software package that needs no additional software routines for operation. The model contains all supporting information necessary for a building analysis except specific user-provided information about the building being analyzed; general supporting information such as weather, fuel costs, and defaults are available directly to the user from a comprehensive data base built into RESEM. RESEM has an easy-to-use interface, providing real-time diagnostic messages to help users recover from input errors, command syntax errors or ambiguities; real-time status messages to keep users informed at all times about the progress of the analysis; and an online help feature that provides context-dependent information based on menu and analysis status when the help request is made. This feature makes written documentation largely unnecessary.

Although only a minimum of information specific to a given building need be input, RESEM can provide a detailed description of any or all aspects of the building when detail is necessary for the most accurate estimates of ECM savings. At any level of input detail the interface shows users explicitly what input parameters are defaulted, what the default values are, and allows users to selectively alter these defaults for the analysis.

RESEM knows all 74 ECM types recognized in the ICP program, and codified in the Grant Tracking System (GTS). Input screens for each ECM type allow a detailed description of the ECM, accurately reflecting design changes to a retrofitted building.

Users can automatically generate verification summaries of all inputs; analysis status during the analysis process; and analysis results including pre-and post-retrofit energy use broken out by end-use and fuel type, retrofit savings for each ECM, and economic measures of ECM performance. Future RESEM development will provide a "Performance Profile" of the building energy consumption and savings (comparing these to average data for an entire class of similar buildings) and an aggregation capability that will allow for total savings realized over a given period in various geographical regions and subregions, building types, and retrofit types.

CORPS OF ENGINEERS' EFFICIENT BUILDINGS

The U.S. military has significantly reduced energy consumption in the past ten years through increasingly stringent energy use standards. DOD standards are a straightforward performance standard, whereas the new DOE energy standards applying to all federal (including military) buildings are both prescriptive and performance standards. The Army Corps of Engineers would prefer to retain DOD standards because they are familiar, easier to apply, and the Corps believes the DOD standards are more stringent than the new DOE standards. The Corps asked LBL to establish whether the DOD standards exceed those of DOE. If so, compliance with the DOD standards would simultaneously meet DOE standards.

Six standard buildings were compared (barracks, battalion HQ, chapel, child care center, warehouse, and maintenance facility), developing a reference building for each according to the DOE procedure. This required application of prescriptive DOE standards to a building of the

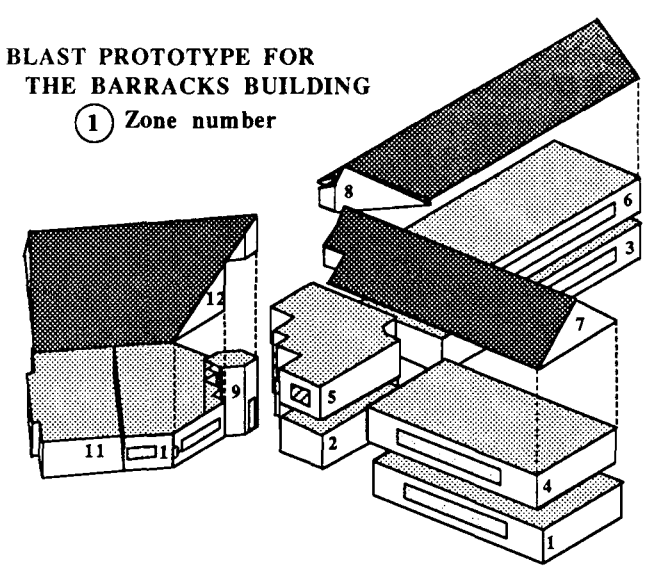


Figure 2. Detailed Zoning for Simulation of Standard Barracks. (XBL 8812-4339)

same type, size, and height as the building under investigation. A BLAST simulation was then run to calculate an energy budget which DOE would allow for that building. This budget was then compared to the DOD energy budget. This was done for six climate regions.

For three of the buildings, the DOD standards always implied compliance with the analogous DOE standards. For two other buildings, the DOE standards were slightly better in only two climates. For the remaining building—the child care center—DOE standards required considerably lower energy use in several climates.

We plan to examine more closely the two buildings that have marginal differences in the standards to determine whether these differences are within the range of uncertainty of DOE procedures and therefore effectively equivalent. The child care (school) building type will be investigated to determine whether the DOD standards must be improved or whether the DOE standards for schools are unrealistic.

Other work will include a life-cycle cost analysis of two building types to determine optimum insulation levels. A set of BLAST input "templates" will be prepared for typical DOE building types to make application of the DOE standards easier for those using BLAST for federal buildings or for other buildings to which DOE standards might apply.

Absorption Heat Pumps*

M. Wahlig, J. Rasson, and M. Warren

Research has continued on development of high-efficiency thermally driven chillers and heat pumps that use *regenerative* absorption cycles. Constant-temperature (instead of constant-pressure) input and output conditions allow regenerative cycles to achieve higher efficiencies than do most (or all) other classes of absorption cooling cycles.

In previous years, simplified calculational methods predicted that a double-effect regenerative (2R) absorption-cycle chiller would operate at about 55%—and a single-effect regenerative (1R) absorption chiller at about 70%—of the ideal Carnot coefficient of performance (COP). Because these cycles are well suited to variable input temperatures between 180 and 280°F, they were explored with solar cooling applications in mind. A 2R chiller was built and tested, and it attained the predicted performance.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Solar Heat Technologies, Solar Buildings Technology Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098; the Department of Engineering Research, Pacific Gas and Electric Company under Contract No. Z19-5-269-87; and the Oak Ridge National Laboratory under Contract No. 10X-SB315V.

Previous work had also identified a gas-driven regenerative cycle configuration, called an absorber-coupled double-effect regenerative (ADR) cycle, that could attain a higher efficiency than the 1R cycle by taking advantage of the high, constant temperature of a gas source.

During FY 1988, we continued development of simulation models that would enable calculation of the performance of high-efficiency absorption-cycle chillers and heat pumps that use ammonia-water as the working fluid pair (work supported by the DOE/Solar Buildings Program as part of a joint U.S./Israel project). We also calculated the detailed performance of a 1R-cycle heat pump over a full range of operating conditions (work supported by the DOE/Buildings Conservation Program, through the Oak Ridge National Laboratory). In addition, we calculated the performance and made an initial estimate of the manufacturing cost of an ADR heat pump (work supported by the Pacific Gas and Electric Company (PG&E) and the Gas Research Institute through PG&E).

The public-domain chemical process flowsheet simulator ASPEN (Advanced System for Process Engineering), selected as the basic tool for modeling the absorption cycles, had been successfully adapted to simulate the 2R cycle. In FY 1988, ASPEN was further modified to simulate the more complex 1R cycle. Convergence problems (in initial attempts to model certain 1R components) were overcome, and the full 1R cycle was simulated successfully.

An in-house, LBL-developed simulation technique (HPSIM) had been developed during FY 1987 to simulate absorption cycles. Although not as comprehensive as ASPEN in its computational ability, HPSIM uses far less computer storage capacity and run time. HPSIM uses a combined simultaneous equation-iterative solution method, using the solver HYBRID. In FY 1988, after the modification of ASPEN for modeling the 1R cycle was completed, the 1R performance predictions of the ASPEN and HPSIM models were found to agree within $\pm 2\%$.

The HPSIM model was then used to calculate the performance of the 1R cycle for different configurations and operating conditions. In particular, the number of pressure steps in the 1R cycle could be reduced from seven to four with a decrease of only about 4% in the cooling COP. Further reduction to three pressure steps reduced the COP another 10%. These results showed that a substantial reduction in cycle complexity (and therefore in manufacturing cost and operating reliability) is possible with only a small decrease in cycle efficiency. The four-pressure-step 1R cycle was calculated to operate at about 65% of the Carnot COP over the full operating range.

The design of the ADR-cycle heat pump was modified to simplify considerably its manufacture and reduce its cost, only modestly reducing its efficiency. Because the ADR cycle uses a higher input temperature than does the 1R cycle, the efficiency of the ADR cycle is expected to be less sensitive to the number of pressure steps. This was confirmed in simulations of ADR cycle performance using the HPSIM model. Reduction from seven to three pressure steps resulted in a negligible decrease in the cooling COP over the full range of operating conditions. A

further reduction to two pressure steps produced a COP reduction of 10–15%.

We then calculated the expected performance of a three-pressure-step ADR heat pump for a full range of cooling-mode and heating-mode operating conditions. At standard ARI rating conditions, the cooling-cycle COP is about 1.69 using water-cooled operation and about 1.35 using air-cooled operation. The heating-cycle COP is about 2.13 at 47°F outdoor temperature, and about 1.66 at 17°F outdoor temperature. These are cycle COP values and do not include combustion efficiency or parasitic electric power for the pumps or fans.

A "first-cut" manufacturing cost study was conducted by Pioneer Engineering and Manufacturing Company for a four-pressure-step ADR heat pump. Detailed cost estimates were made for the new heat exchangers unique to the ADR heat pump design, and existing cost estimates were used for components common to other heat pumps operating at the same pressures and using ammonia as the refrigerant. A rough estimate for the solution pump cost was based on available information, resulting in an estimated total manufacturing cost of about $1550 for a 3-ton ADR heat pump. A similar cost study for a three-pressure-step design would be expected to result in a slightly lower cost. Iteration in design detail could also have a substantial effect on reducing manufacturing cost.

A primary objective of the joint U.S./Israel project being conducted by the Technion and LBL is to develop a simulation model suitable for all types of absorption chiller and heat pump cycles. Initial attention is being focused on the generator-absorber heat exchange (GAX) cycle because it is likely to be the first advanced absorption cycle to be available commercially and is therefore a candidate for being driven by evacuated-tube solar collectors that can operate efficiently up to 400°F.

Accordingly, the Technion and LBL are using separate calculations of GAX cycle performance as a measure of agreement between the various computer models for absorption cycles. The intention is to combine the best solution methods into a single computer model, which will most likely be an improved version of the user-friendly model originated by the Technion group. The GAX cycle was successfully simulated at LBL using HPSIM, and intercomparisons of LBL and Technion results of GAX cycle simulations—as well as resolution of any differences that may occur using different models—are expected to take place during FY 1989.

Simulation Research*

F.C. Winkelmann, B.E. Birdsall, W.F. Buhl, K.L. Ellington, A.E. Erdem, J.M. Nataf, and E.F. Sowell[†]

The Simulation Research Group (SRG) has the long-term objective of providing the architectural, engineering, and research communities with software tools to assist in the design of energy-efficient, cost-effective buildings. The ongoing research of the SRG has two main focuses: 1) to develop and maintain the current-generation benchmark program (DOE-2), and 2) to develop the next generation of building performance calculation tools (the Energy Kernel System).

DOE-2 is a public-domain computer program which, given a description of a building's climate, architecture, materials, operating schedules, and HVAC equipment, performs an hour-by-hour simulation of the building's expected energy use and energy cost. DOE-2 is widely used in the United States and 35 other countries to design energy-efficient buildings, analyze the impact of new technologies, and to develop energy conservation standards. Details of the development and structure of the DOE-2 program are available.[1–11]

The Energy Kernel System will provide basic tools and information to allow SRG and other groups to develop future simulation programs. It will also provide a mechanism for exchanging research results and technology advances, and a basis for integrating performance simulation into computer aided design (CAD) and expert system software.

DOE-2

SRG maintains a research effort to develop enhanced versions of DOE-2. This ongoing research is divided into three parts: 1) introduction of algorithm description techniques into the code; 2) modeling of building envelope components and systems; and 3) simulation of HVAC equipment and associated control systems. The next version of the program, DOE-2.1D, is scheduled for public release in FY 1989. Several major new features follow:

User-Defined Functions. A new FUNCTION command added to the DOE-2 SYSTEMS program permits modification, enhancement, or replacement of DOE-2 calculations without recompiling the program. Users write

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division of the U.S. Dept. of Energy under Contract No. DE-AC03-76SF00098.

[†]Visiting scientist. Permanent address: Department of Computer Science, California State University at Fullerton, Fullerton, California.

their own algorithms in a FORTRAN-like language and place this information in their input, along with information indicating how and where the new algorithms are to be used. This feature allows researchers to add new HVAC simulation features, such as innovative control schemes, that could not be modeled by the regular DOE-2 calculations.

Generalized Library. A new library feature allows DOE-2 users to create custom libraries containing descriptions of any building component or system of components. Libraries may be defined to contain such data as room geometry, standard operating schedules, or frequently used HVAC system descriptions. This feature will greatly simplify input preparation.

Improved Fenestration Calculation. Because heat gain and loss through windows greatly affects the energy performance of most buildings, DOE-2 window thermal calculations are being improved to calculate automatically the shading of diffuse solar radiation by neighboring buildings and by architectural elements such as overhangs (previously only the shading of direct solar radiation was calculated); to more accurately calculate skyward infrared radiation loss from the building envelope, taking into account atmospheric conditions and architectural obstructions; and to more accurately calculate the amount of sky diffuse radiation falling on windows and walls.

Desiccant Cooling. In most climates, occupant comfort during warmer months requires that room air be dehumidified. Several companies are developing desiccant cooling systems in which a hygroscopic material such as lithium bromide removes moisture from the supply air stream. The desiccant is "regenerated" for further use by drying it with hot air from a gas-fired heater. Gas-fired desiccant systems of this type can replace or supplement conventional electric-driven cooling systems; however, almost nothing is known about the economics of desiccant systems for different climates, building types, and utility rate structures. For this reason, SRG (with funding from the Gas Research Institute via the GARD Division of the Chamberlain Manufacturing Corporation) is creating DOE-2 models to simulate the performance of a variety of desiccant systems currently under development. GRI will use these DOE-2 models to identify the most cost-effective desiccant cooling schemes.

Advanced Simulation

In recent years, the search for more efficient building designs has led to components, systems, and whole building structures which are extremely complex and therefore difficult to analyze. Because existing programs like DOE-2 were initially conceived in an era when design questions were much simpler than they are today, the analytic capabilities of these programs are fundamentally limited. Generalized, computationally efficient, easily extendible techniques are needed to accurately simulate the interactions' between building-envelope components and HVAC equipment. Analysis of complex designs and advanced technologies requires substantially improved building performance simulation programs. To continue to meet DOE's long-term objective of providing up-to-date and reliable analysis tools, basic research has begun into new simulation techniques. This work will lead to replacement of DOE-2 with a tool designed to meet the needs of architects and engineers in the 1990's.

An international collaborative effort between SRG and research groups in the U.K. has been initiated to produce the new software. This effort will provide not only a significant advance in building performance simulation but also a mechanism for communicating and exchanging results among diverse communities of designers and researchers.

Within the general goals and structure of the advanced simulation software,[12–15] the primary goal is to provide a software environment (the **Energy Kernel System** or **EKS**) for developing new simulation programs. This environment would allow a high level of model construction flexibility and facilitate state-of-the-art integration of new techniques with old. Other goals are to permit different modeling approaches, to encourage collaboration among model developers, and to take advantage of emerging software engineering in the area of multiprocessing.

The EKS (Figure) will consist of 1) a library of software modules or *objects* representing different building components, physical processes, and mathematical solution techniques, and 2) an executive program or *harness* which allows users to link software objects to form customized energy models. The EKS user will first construct a *template* which defines a model as a collection of objects and a set of messages controlling the order of execution of the objects and the flow of information among them. The template is used by the harness to construct the final program in the form of source (or executable) code.

The EKS is designed for use by model *developers*, not by model users. It is intended to be an efficient way of creating simulation models that can be used in a stand-alone fashion or for integration into multipurpose environments such as computer-aided design (CAD) systems, expert systems, or energy management systems.

SPANK: A Prototype Energy Kernel System. In FY 1986 the SRG began developing new software called the Simulation Problem ANalysis Kernel (SPANK) as a first prototype of the EKS.[16,17] SPANK views a simulation problem as a network — the nodes represent nonlinear equations, and the lines linking the nodes (called links or arcs) represent variables in the equations. The network representation of a simulation problem is completely equivalent to describing the problem as a set of simultaneous, nonlinear algebraic and differential equations. The network representation allows use of graph theory techniques to reduce the size of the problem to be solved.

A simulation problem in SPANK consists of a set of coupled equations. Each equation or relation among variables is known as a *primitive object*. Primitive objects may be combined into *macro objects*, and primitive and macro objects can be combined into more complex macro objects. Thus modules (sets of equations) which represent complicated physical processes or entities can be built up

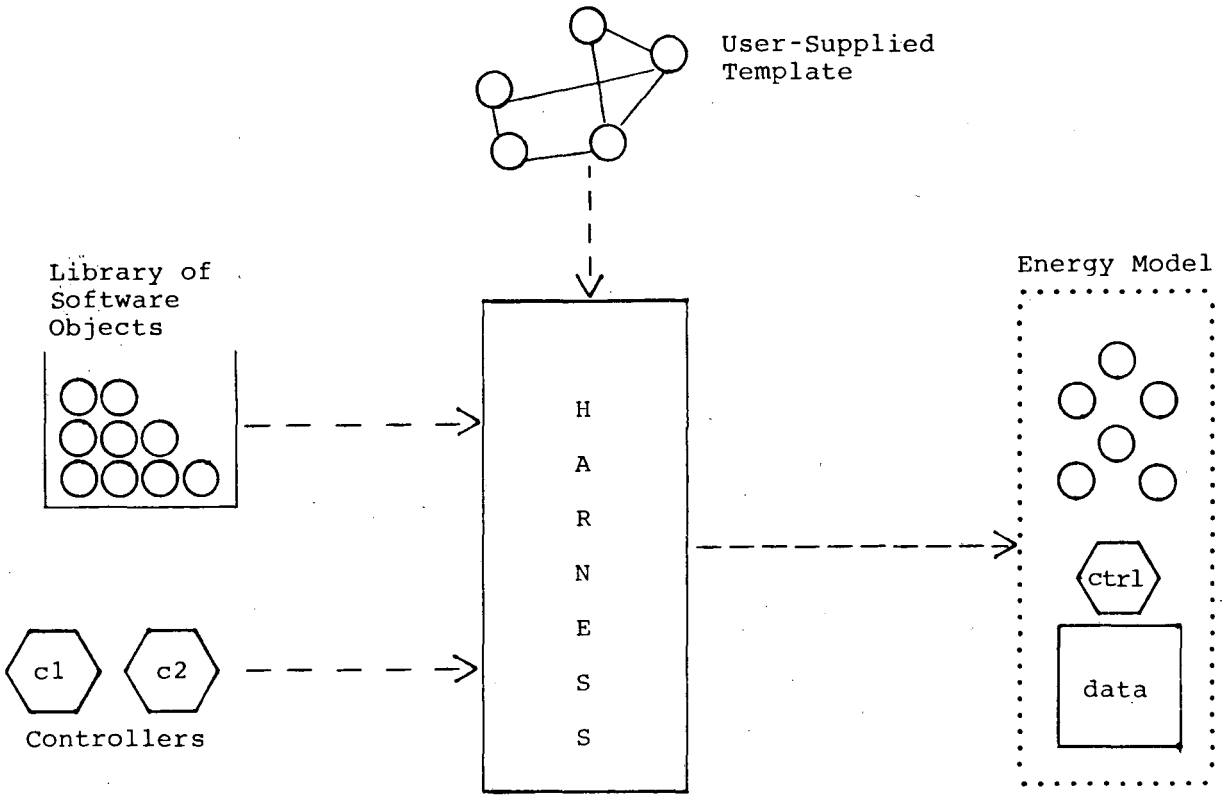


Figure 1: Proposed Energy Kernel System for creating building energy simulation models. (XBL 8712-5767)

from simple components. After the necessary objects (simple or complex) are defined, the problem description is completed by "linking" the objects together, i.e., by specifying the variables common to given equations.

Users need only define the simulation problem and do not need to choose a computation sequence (e.g., write a procedural algorithm in FORTRAN or other language) to solve the set of equations.

SPANK creates the solution sequence in two steps. First, a particular relationship (equation) is selected for each variable and inverted to give a formula for that variable. After the matching is accomplished, the second step is to find a set of break variables—a *cut set*. that become the iteration variables in the solution sequence. (Initial values are guessed and then used to solve for all the variables using the set of relationships. This procedure yields new values for the cut set variables. A scheme such as Newton-Raphson iteration is then used for choosing the next guess for the cut set.)

When faced with solving a system of nonlinear equations, most simulation programs simply iterate on all the variable, i.e., the cut set includes all variables in the problem. One of SPANK's major contributions is to use graph theory methods to reduce the cut size greatly and thus effectively reduce the problem size.

In FY 1988, object-oriented techniques were developed to allow SPANK to simulate time-dependent processes by integrating first-order differential equations.[18]

In FY 1988, we will continue to maintain and support the DOE-2 program and to publish the quarterly *DOE-2* User News. An improved version of the program, DOE-2.1D, will be completed and released to the public.

The SPANK program will be released for outside review after in-house testing of new SPANK features, including a graphics-based input processor, dynamic simulation, and symbolic manipulation of objects. Detailed specifications for the EKS will be developed.

REFERENCES

1. LBL Simulation Research Group, *DOE-2 Supplement, Version 2.1C*, LBL-8706 Rev. 4., 1984, Suppl.
2. LBL Simulation Research Group, *DOE-2 BDL Summary, Version 2.1C*, LBL-8688 Rev. 4, 1984.
3. LBL Simulation Research Group, *DOE-2 Users Guide, Version 2.1A*, LBL-8689 Rev. 3, 1981.
4. LBL Simulation Research Group, *DOE-2 Sample Run Book, Version 2.1C*, LBL-8678 Rev. 2.
5. LBL Simulation Research Group [LBL] and Group Q-11 [LANL]. *DOE-2 Reference Manual, Version 2.1C*, LBL-8706 Rev. 4, 1984.
6. Diamond SC, Hunn BD. *DOE-2 Verification Project: Phase 1, Interim Report*, LANL Publication LA-8295-MS, 1981; Diamond SC, Capiello CC, Hunn BD.

DOE-2 Verification Project: Phase 1, Final Report, LANL Publication LA-10649-MS, 1986.

7. Hirsch JJ. *Simulation of HVAC Equipment in the DOE-2 Program*, LBL-14026, 1982.
8. Simulation Research Group. *Overview of the DOE-2 Building Energy Analysis Computer Program*, LBL-19735, 1985.
9. Simulation Research Group [LBL] and Group Q-11 [LANL]. *DOE-2 Engineers Manual, Version 2.1A*, LBL-11353 and Los Alamos National Laboratory Publication LA-8520-M, 1982.
10. Winkelmann FC, Selkowitz S. Daylighting Simulation in the DOE-2 Building Energy Analysis Program, *Energy and Buildings, 1986; 8:271.*
11. Buhl WF, Erdem AE, Eto JH, et al. *New Features of the DOE-2.1C Energy Analysis Program*, LBL-19870, 1985.
12. Buhl WF, Erdem AE, Hirsch JJ, et al. *A Proposal to Develop a Kernel System for the Next Generation of Building Energy Simulation Software*, Lawrence Berkeley Laboratory, 1985.
13. Hirsch JJ. *Plan for the Development of the Next Generation Building Energy Analysis Computer Software*, LBL-19830, 1985.
14. Clarke JA, Hirsch JJ, Buhl WF, et al. Planned Developments in Building Energy Simulation. In: *Proceedings of the 5th CIB Symposium on Energy Conservation in the Built Environment*, Bath, England, 1986.
15. Winkelmann FC. Advances in Building Energy Simulation in North America, *Energy and Buildings* 1987; 11:161.
16. Anderson JL. *Network Definition and Solution of Simulation Problem*, LBL-21522, 1986.
17. Sowell EF, et al. Prototype Object-Based System for HVAC Simulation. In: *Proceedings of the Second Systems Simulation Conference*, Liege, Belgium. LBL-22106, 1986.
18. Sowell EF, Buhl WF. *Dynamic Extension of the Simulation Problem Analysis Kernel.* LBL-26262, 1988.

WINDOWS AND LIGHTING PROGRAM STAFF

Stephen Selkowitz, Program Leader

Dariush Arasteh
Erica Atkin
Charles Benton
Samuel Berman*
Carolann Caffrey
Mark Cavanagh
Robert Clear
Douglas Crawford
Dennis DiBartolomeo
Marc Fountain
Ellen Gailing
Ann Hatcher
Mary Lou Hinman
Donald Hollister
John Hutchins
Richard Johnson
Harry Keller
Guy Kelley
Jong Jin Kim
Joseph Klems
Steven Lambert
Carl Lampert
Donald Levy
Fuzi Li†
Anne McClintock
Cherise Morris
Oliver Morse‡
Manfred Neiger†
Werner Osterhaus
Konstantinos Papamichael
Susan Petersen
Susan Reilly
Robert Richardson†
Michael Rubin
Francis Rubinstein
Jennifer Schuman
Stephen Selkowitz*
Masanori Shukuya†
Michael Siminovitch
Robert Sullivan
Rudy Verderber
Gregory Ward
Richard Whiteman§
Michael Wilde
Ruth Williams
John Wolfe
David Wruck
Mehrangiz Yazdanian
Edward Yin

*Group Leader
†Participating Guest
‡Plant Engineering
§Engineering Division

WINDOWS AND LIGHTING PROGRAM

INTRODUCTION

Over 30% of all energy used in buildings is attributable to two elements: windows and lighting. Together they account for annual consumer expenditures of over $50 billion. Each affects not only energy use by other major building systems but also comfort and productivity, factors that have a far greater influence on building economics than direct energy consumption alone. Windows play a unique role in the building envelope, physically separating the conditioned space from the world outside without sacrificing vital visual contact. Lighting systems facilitate a variety of tasks with a wide range of visual difficulty throughout the indoor environment while defining the luminous qualities of the indoor environment. These two building elements are thus essential components of any comprehensive building science program.

Despite important achievements in reducing building energy consumption over the past decade, significant additional savings are still possible. These will come from two complementary strategies: 1) better building designs that effectively apply existing technology and extend market penetration, and 2) new advanced technologies to increase the savings potential of each application. Both the Windows and Daylighting Group and the Lighting Systems Research Group have made substantial contributions in each of these areas. The ongoing research described in the annual summary aims to further advance achievement of these goals.

The **Windows and Daylighting Group** focuses on developing the technical basis for understanding and improving the energy-related performance of windows. If the flow of heat and light through windows and skylights can be properly filtered and controlled, these building elements can outperform any insulated wall or roof component and provide net energy benefits to the building. The group's investigations are designed to develop the capability to accurately predict net fenestration performance in residential and commercial buildings. Simulation studies, field measurements in a mobile field test facility, and building monitoring studies help us to understand the complex tradeoffs in fenestration performance. The research program is conducted with the participation and support of industry, utilities, universities, design professionals, and government. The Group's three major project areas are optical materials, fenestration performance, and building applications and design tools.

In our studies of optical materials and advanced concepts, we develop and characterize thin-film coatings and other new optical materials that control radiant and thermal flows through glazings. Innovative concepts for large-area envelope enclosures are studied. The program helped accelerate the development and market introduction of windows incorporating high-transmittance, low-emittance (low-E) coatings for R3-R5 windows. If sales follow current trends, by the year 2000 these coatings will save consumers over $3 billion annually in heating bills alone.

Our research on window performance aims to develop new analytical models and experimental procedures to predict the thermal and solar-optical properties of the complex assemblies of glazing materials and shading devices that compose complete fenestration systems. Thermal performance models are being validated with the Mobile Window Thermal Test (MoWiTT) Facility, now collecting data at a field test site in Reno, Nevada. This unique facility combines the accuracy and control of lab testing with the realism and complexity of dynamic climatic effects. LBL daylighting studies employ a unique 24-foot-diameter sky simulator (for testing scale models under carefully controlled conditions), and new experimental facilities for measuring the photometric and radiometric properties of complex fenestration systems.

Building applications studies and design tools help us to understand the complex tradeoffs in fenestration performance as a function of building type and climate. In nonresidential buildings, major reductions in electric energy use and peak electric demand can be achieved if the tradeoffs between daylight savings and solar-induced cooling loads are understood. We are developing concepts for an Advanced Envelope Design Tool using new imaging techniques and expert systems.

The research of the **Lighting Systems Group** is divided into three major areas: advanced light sources, building applications, and impacts on productivity and health.

Our research on advanced light sources is concerned primarily with developing new technical concepts for efficiently converting electrical energy into visible light. Areas of interest include mechanisms for reducing ultraviolet self-absorption in gas-discharge lamps and excitation of the lamp plasma by radio frequency (RF) electromagnetic fields. Both areas promise more efficient conversion of electrical energy into visible light, and possibly much longer lamp life.

Our building applications research concentrates on design of lighting systems, effective use of lighting controls, and how these factors interact with a building's HVAC system.

Research in visibility concentrates primarily on gaining basic information needed to define lighting conditions that enhance productivity in a cost-effective

manner. We also seek to determine any possible undesirable visual effects such as visual fatigue, related to glare and lighting, especially as these events affect the automated workplace.

Our studies of health impacts extend electric lighting research to a wider class of human activities. In a specially designed experimental room, lighting conditions are controlled and human responses are measured objectively by sensitive instrumentation.

The Lighting Group's successes include advancing the development of high-frequency solid-state ballasts for fluorescent lamps and the invention of a new high-frequency surface wave lamp with 30% better efficiency than the common fluorescent lamp. A 2-year test of solid-state ballasts in a large office building showed an electricity savings of 40%. Scaled to the entire country, this represents an annual savings of $5 billion. The energy-efficient surface wave lamp promises major reductions in energy use with considerably longer lamp life.

Windows and Daylighting*

S.E. Selkowitz, D. Arasteh, C. Benton, D.L. DiBartolomeo, R.L. Johnson, J.J. Kim, J.H. Klems, C.M. Lampert, K. Papamichael, M.D. Rubin, R. Sullivan, and G.M. Wilde

Approximately 20% of annual energy consumption in the United States is for space conditioning of residential and commercial buildings. About 25% of this amount is required to offset heat loss and gain through windows. In other words, 5% of U.S. energy consumption—the equivalent of 1.7 million barrels of oil per day—is tied to the performance of windows. Fenestration performance also directly affects peak electrical demand in buildings, sizing of the heating, ventilating, and air-conditioning (HVAC) system, and the thermal and visual comfort of building occupants, as well as their health and productivity.

With more intelligent use of existing technology and with development of new high-performance window materials, windows can be converted from energy liabilities to energy benefits. The aim of the Windows and Daylighting Group is to develop the tools and technologies to accomplish this goal. Research is required to develop the new technologies and capabilities to predict and improve the thermal, energy, and daylighting performance of windows and skylights. The group's work helps generate guidelines for design and retrofit strategies in residential and commercial buildings and contributes to development of advanced computer-based tools for building design.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Systems Division, and Office of Solar Heat Technologies, Solar Buildings Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Our program's strength lies in its breadth and depth: we examine energy-related aspects of windows at the atomic and molecular level in our materials science studies, and at the other extreme we perform field tests and in situ experiments in large buildings. We have developed, validated, and now use a unique, powerful set of computational tools and experimental facilities. Our scientists, engineers, and architects work in collaboration with researchers in industry and academia.

To be useful, the technical data developed by our program must be communicated to design professionals, industry, and others in the public and private realms. We publish our results and participate in industrial, professional, and scientific meetings and societies, national and international, to ensure that our research results are widely disseminated and utilized.

Our research is organized into three major areas:

- Optical Materials and Advanced Concepts
- Fenestration Performance
  - —Thermal analysis
  - —Daylighting analysis
  - —Field measurement of performance
- Building Applications and Design Tools
  - —Nonresidential buildings
  - —Residential buildings
  - —Design tools

OPTICAL MATERIALS

Significant reductions in energy consumption of buildings will come not only from better building design, but also from the development and introduction of new glazing materials. Since the inception of our program in 1976, we have worked to identify, characterize and develop promising new optical materials to assist industry with developing the next generation of advanced fenestration systems. We also provide scientific coordination for DOE-funded research projects at universities, private-sector firms, and other national laboratories, and work to transfer our research results to the private sector.

In 1976, we made the development of low-emittance (low-E) coatings a major program objective, and our DOE-supported research subsequently accelerated market introduction of high-performance low-E window systems. Several small firms began offering commercial products in 1982, and by 1985 most of the largest glass and window manufacturers offered low-E products. Incorporating low-E coatings into conventional double-glazed windows produces a lighter, more compact unit with better thermal performance than triple-glazed windows. Ultimately windows using this coating technology could have heat transfer values as low as those of insulating walls, and save more energy annually than the best-insulated wall.

DURABLE LOW-EMITTANCE COATINGS

The objective of this project is to develop a second-generation low-E coating with high transmission and clarity that will last for the lifetime of a window. Among low-E coatings made today, those based on sputtered

silver have the best optical properties and lowest emissivity. Silver, however, is a soft metal and is subject to agglomeration and loss of optical quality. We began by studying titanium nitride, a material that combines optical properties similar to those of a noble metal with the mechanical and chemical durability of a ceramic. Using advanced deposition techniques and multilayer design, we were able to produce coatings with properties exceeding those of the best commercial coatings. This year we began investigating diamond-like films for use as protective and antireflection layers for metallic low-E coatings. The first task was to deposit diamond-like films using standard industrial sputtering technology. These films tend to have low transmittance in the visible spectrum; we were able to increase transmittance by varying the deposition parameters. Figure 1 shows the beneficial effect of reducing sputtering power on the transmittance of diamond-like films. Next year we will continue to optimize the optical properties of diamond-like coatings on silver and test their durability in collaboration with industrial partners.

LOW-CONDUCTANCE GLAZINGS

With the commercial success of R3-R4 windows incorporating coatings and gas-filled insulated glass (IG) units, the next major challenge lies in increasing the R-value of windows' center-of-glass, edge-of-glass, and frame areas. In FY 88 we continued to develop our concept for a high-R window that can be manufactured using existing industrial production facilities. This high-R window is based on an innovative modification of conventional triple glazing. Two low-E coatings are placed on surfaces facing each of two krypton- or krypton/argon-filled gaps. Such a design can achieve center-of-glass R-values between 6 and 10. However, the use of conventional metal spacers to separate the glazing layers creates a large two-dimensional thermal bridge at the outer edge of the IG unit. Furthermore, even the best wood frame will degrade the thermal performance of such a window.

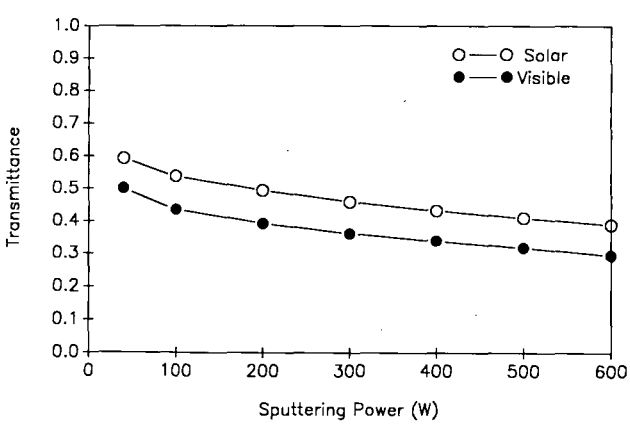


Figure 1. Total solar and visible transmittance versus fraction of H_2 flow in the Ar/H_2 mixture at 200 W. (XBL 892-643)

This year we collaborated with four major window manufacturers to design prototype high-R windows for demonstration home projects set up by electric utility companies in Montana and Wisconsin. Frame and edge designs were modified to reduce heat transfer in these areas. Field monitoring and MoWiTT testing of these windows is planned for FY 89. This work was supported by the Bonneville Power Administration and the Wisconsin Power and Light Company, as well as the U.S. DOE.

OPTICAL SWITCHING MATERIALS

Optical switching materials can be used to dynamically regulate the transmission of windows in buildings and automobiles. Initial studies of energy simulation of office buildings indicate that an automatically controlled switchable coating can provide substantial energy savings in lighting and cooling as well as economic benefits in reduced HVAC system size. The transmittance of a window can be controlled either by electrochromic, thermochromic, photochromic, or liquid crystal materials. Electrochromic devices appear to have the best combination of properties for window applications, including a wide-dynamic visible transmittance range (possibly 8:1 transmittance change), moderately fast switching times, and low power consumption.

During FY88 we developed component layers for the fabrication of devices. The component layers consist of the following materials: 1) electrochromic, 2) ionic electrolyte/conductor, and 3) ion storage. All of our devices are based on electrochromic nickel hydroxide. The best nickel hydroxide layers are deposited by anodic electrochemical deposition using sulfate/nitrate solutions developed by our group. In addition we have made films of nickel hydroxide and vanadium oxide by reactive d.c. sputtering. The optical and electrochemical properties of the films have been investigated using optical spectroscopy and cyclic voltammetry. We have synthesized a quarternary ammonium hydroxide polymer for use as an electrolyte in the device. This polymer has ionic conductivity of 8×10^{-2}S/cm. Devices using this polymer exhibited an integrated photopic response of 70-21% between bleached and colored states (Figure 2).

Our research in FY 89 is directed at improving the durability of the polymer electrolyte, altering the oxidation potential of nickel hydroxide by doping, and developing ion storing electrodes with compatibility to nickel hydroxide. Materials we will study for ion storage include manganese and niobium oxide. To simplify analysis, we will develop computer controlled instrumentation to perform in situ optical and electrochemical experiments.

CORE DAYLIGHTING SYSTEM DESIGN

Outdoor illuminance levels under clear skies are typically 100 times greater than required indoor illuminance levels. If just a fraction of the sunlight falling on a building could be distributed to core building zones, daylight could offset a building's entire electric lighting load during sunny periods, with automatically dimming electric

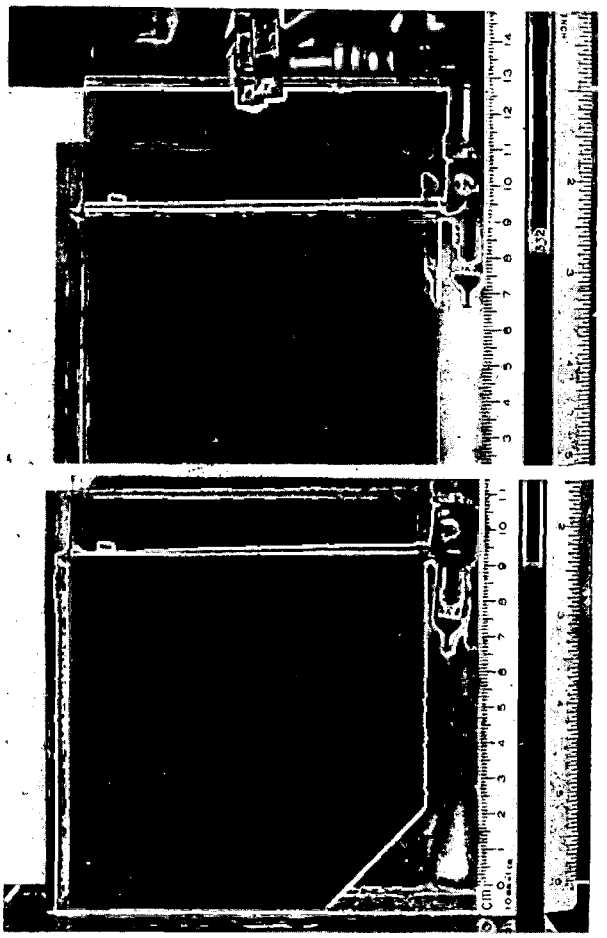


Figure 2. Electrochromic nickel oxide device shown in its colored and transparent states. (CBB 887 6776A)

luminaires providing light at other times. Several core daylighting systems have been developed, and one Japanese system is in commercial production, but these systems are not cost-effective on the basis of their energy savings. We have developed a new design, however, that could supply daylight to core building zones with a cost-effective optical technology.

Our previous work showed that direct sunlight can be channeled to core building zones through light guides small enough for retrofit as well as new-building applications. To attain this level of optical concentration, the system would use tracking solar collectors maintaining stringent tracking and optical imaging tolerances. A practical and economical collector design to achieve these tolerances was developed in FY 87. During FY 88 we developed an algorithm for optimizing the collector's mechanical design; analyzed the radiative heat gain in the system's plastic optical fiber elements and concluded that with proper design thermal gains would not exceed the fibers' thermal tolerance limit; refined the optical theory underlying the collector's Fresnel lens design and filed an initial patent application for a mechanism that substantially eliminates chromatic dispersion in the lens; and developed software for completing the optical design for the overall core daylighting system.

We will continue developing the collector's optical and mechanical design and will refine our estimates of the system's performance characteristics, cost parameters, and projected energy savings. Since subjective response to the interior environment is an important element in overall system design and cost effectiveness, we will consider using the Radiance program to evaluate the system's illumination quality and its interaction with dimmable electric lighting. This software would be used as a design guide not only in the development of core daylighting systems, but also for analyzing new optical component designs for window and skylight applications.

ADVANCED GLAZINGS FOR AUTOMOBILES

Solar heat gain accounts for a large proportion of the cooling loads requiring automobiles to be built with large, high-capacity air conditioners, which in turn release significant amounts of chlorofluorocarbons (CFCs) into the atmosphere. As part of its program to reduce CFC emissions from auto air conditioners, the Environmental Protection Agency supported a study to determine the potential for reducing air conditioner size by using advanced glazing with selective transmittance properties for controlling solar heat gain. Our objective was to define the relative performance of a range of real and hypothetical absorptive and reflective glazings under static-soak and cool-down conditions.

We completed an extensive analysis of the effects of glazing and ventilation options in standard and sports-model sedans by running parametric simulations of a wide range of absorptive and reflective glazing components using a finite-difference computer program. Figure 3 shows the peak interior air temperature under static-soak

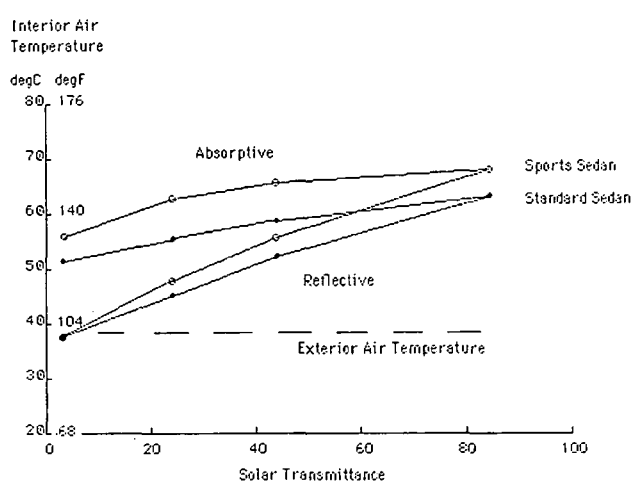


Figure 3. Peak interior air temperatures for standard and sports sedans as a function of solar transmittance. Values occur at 3 p.m. and are shown for reflective and absorptive glazings. (XBL 892-646)

conditions in Phoenix, Arizona, for glazings of varying solar transmittance. The absorptive and reflective curves represent limiting values of these properties. Our final report includes an annotated bibliography of work on solar-load control for automobiles in the form of a hypertext computer program. This gives users quick and easy access to a large volume of data that would otherwise be too cumbersome for convenient use.

Our future work will relate auto air conditioner performance and glazing characteristics to actual fuel use. Although we know that gasoline consumption increases with air conditioner use, the potential for improving fuel efficiency has not been thoroughly studied. We plan to perform analytical and experimental investigations under a variety of driving conditions in several climates. We also expect to begin development of new coating technology to meet the performance requirements we have identified.

FENESTRATION PERFORMANCE

Research activities in this area are intended to characterize the performance of fenestration components and complete systems over the entire range of operating conditions in any climate or building type. The research develops and refines experimental techniques and analytical models for accurately determining heat-transfer and solar-optical properties of fenestration components and systems and validates these models in field-test facilities and occupied buildings. Many of the new algorithms and data sets are designed to be incorporated into hour-by-hour building energy simulation programs such as DOE-2.1. These data not only improve the accuracy of our predictions but also allow us to predict the performance of new fenestration systems and novel architectural designs. Our plan for developing and implementing these new analysis capabilities in energy simulation models is shown schematically in Figure 4.

THERMAL ANALYSIS

With the wide acceptance of low-E coatings and the introduction of low-conductance gases by the window industry, the number of possible window configurations has multiplied rapidly, creating a need for an accurate, convenient, and standard calculational procedure to determine window heat-transfer indices. The Windows and Daylighting Group developed a computer program to fill that need. WINDOW 2.0 was released in 1986 and distributed by LBL and a major window sealant manufacturer as a professional courtesy to over 800 window and IG-unit manufacturers. The program has since become the de facto standard in the industry, and our efforts to develop WINDOW and make it available to the private sector were recognized by the Federal Laboratory Consortium's 1988 Special Award for Excellence in Technology Transfer.

In FY 88 we added many new technical and user-friendly features to an updated version of the program. Users of WINDOW 3.1 have easy access to libraries of component information and can easily build or change a window and see the resultant thermal properties on the same screen. Version 3.1 includes help screens, and its operation is consistent with standard MS-DOS software. WINDOW 3.1 is being distributed by window and sealant manufacturers, and other industry organizations have also expressed interest in distributing this program to their members.

Our early work emphasized center-of-glass U-values, but glass-edge and frame effects are known to be significant, particularly in high-performance windows. We have begun a thermal analysis program to study these two-dimensional heat transfer effects (Fig. 5). Results from these finite-element models will be incorporated into libraries in WINDOW 3.1 in order to give the user heat-transfer properties indicative of complete windows and not just center-of-glass performance. These finite-element models have been used to study pressure and temperature induced stresses in high-performance glazings.

In FY 89 we expect to use thermographic techniques in conjunction with more extensive finite-element modeling to develop and validate the library of sash and frame heat-transfer effects. These tools will also allow us to explore the problems associated with condensation on glass edges and frames.

DAYLIGHT AND SOLAR HEAT GAIN STUDIES

Providing daylight to building interiors is one of fenestration's most important functions, both from an energy perspective and from an occupant's point of view. However, the solar heat gain associated with daylight can be a benefit or cost, depending on circumstances. Analyzing the trade-offs to arrive at an optimum solution for simple glazings is difficult; for complex fenestration with sophisticated sun control systems it is virtually impossible with currently available tools. Our objective is to develop the experimental facilities and analysis models to accurately characterize the daylight and solar heat gain from fenestration systems of arbitrary complexity. We conduct a wide range of activities to establish the facilities, tools, and data to address these problems.

Solar-Optical Properties of Complex Fenestration Systems

A quantitative understanding of the solar-optical properties of fenestration systems is essential to accurately predict their luminous and thermal performance for any sun, sky or ground conditions. "Luminous performance" refers to daylight illuminance and luminance levels that determine electric lighting requirements and visual comfort. "Thermal performance" refers to solar heat gain levels that determine heating or cooling requirements and thermal comfort.

We are developing a method of calculating the solar and daylight transmission through complex fenestration systems from laboratory measurements of the solar-optical properties of window components. The method treats fenestration systems as radiation sources of varying-intensity distribution. For diffusing, diffusely reflecting, or geometrically complex components such as blinds or

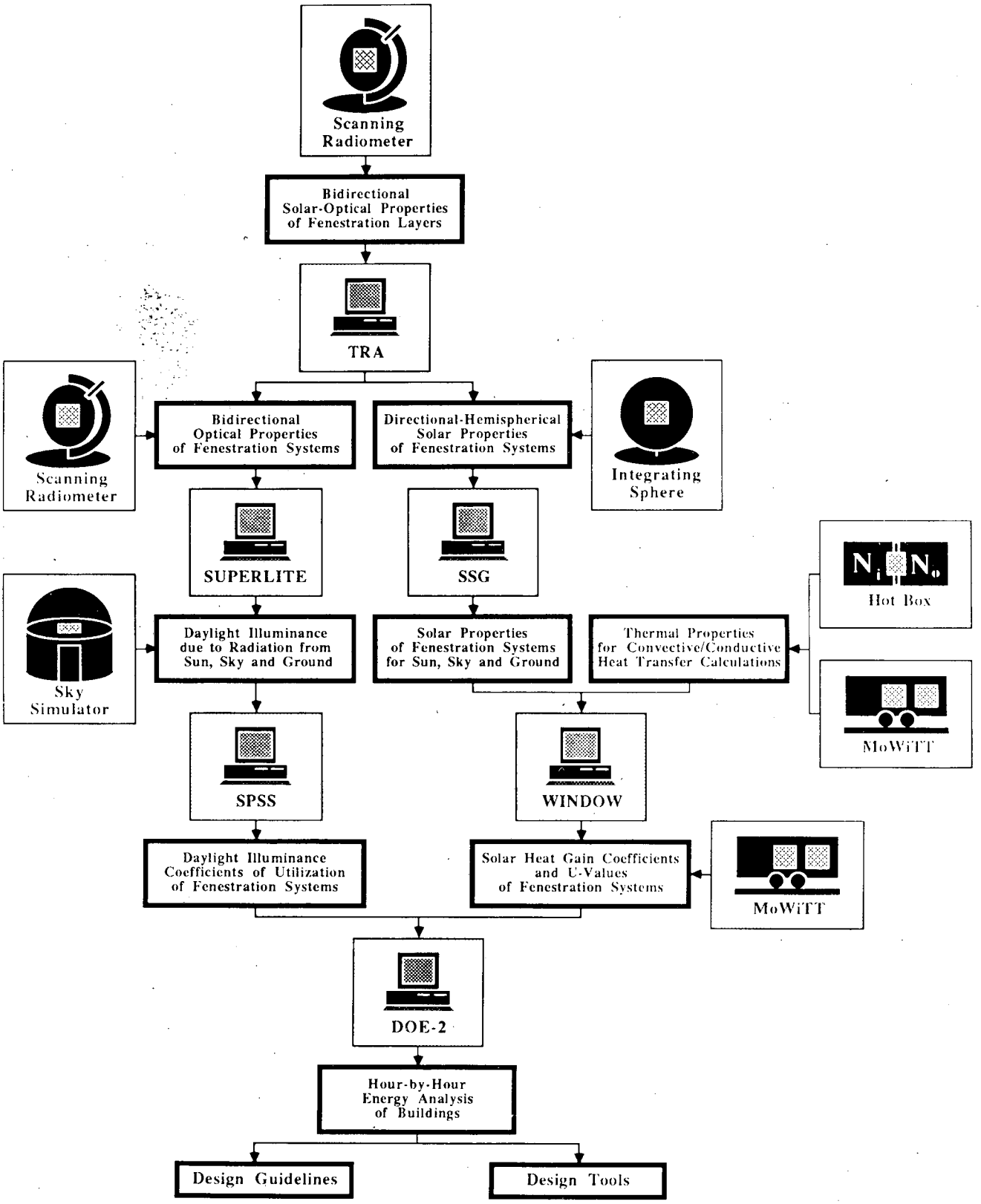


Figure 4. Schematic diagram of overall fenestration modeling capabilities under development includes new measurement facilities, computer models, and intermediate calculated and measured results. Direct measurement of some intermediate calculated results provides a validation check. (XBL 885-1479)

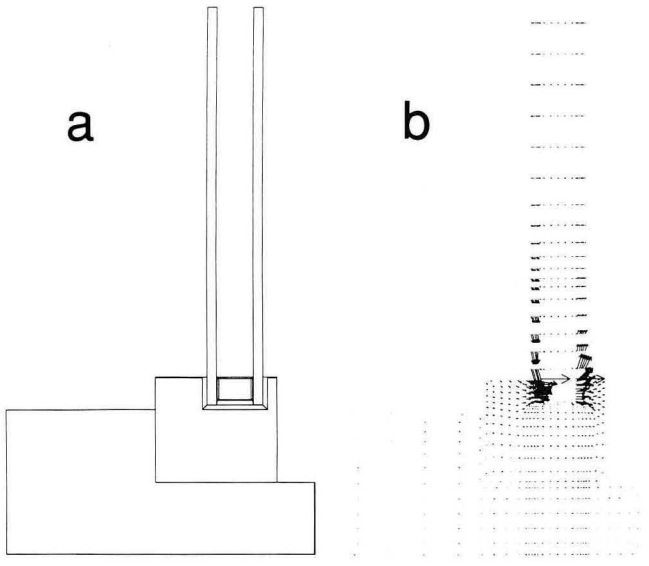


Figure 5. a) Cross section of window edge and frame. Glazing layers are separated by a dessicant-filled metal spacer sealed inside a wood sash that rests on a wood frame. b) Vector plot of two-dimensional heat transfer through the window section shown in (a). Warm interior is at left, cold exterior at right. Size of vector denotes magnitude of heat transfer; arrow denotes direction. All glass two-dimensional heat transfer occurs within the bottom 2.5 inches of glass panes modeled. Small vectors appear as dots. (XBB 892-642)

drapes, bidirectional solar-optical property measurements are necessary. We have developed a large-scale, automated scanning radiometer/photometer to make these measurements (Fig. 6). Computer software will compute the luminous or radiant distribution transmitted by a complete fenestration system for a given set of exterior conditions by combining the properties of component layers while correctly accounting for multiple reflections. During FY88 we initiated a cooperative project with support from DOE and ASHRAE to make this method the basis for a new treatment of solar heat gain through fenestrations. Scanning radiometer measurements will be made on a representative sample of fenestration components, the completed software will be used to calculate the solar heat gain, and the method will be validated by comparison with measurements made with the Mobile Window Thermal Test Facility (MoWiTT).

DAYLIGHTING ANALYSIS

The prediction of lighting quantity and quality in the luminous environment is essential for energy-efficient lighting design. Over the years, we have developed a range of daylighting design tools to expand our modeling capabilities and improve calculational accuracy. Our most advanced daylighting simulation model, SUPERLITE 1.0, was converted to run on an IBM-compatible personal computer in FY88. We continued our efforts to expand

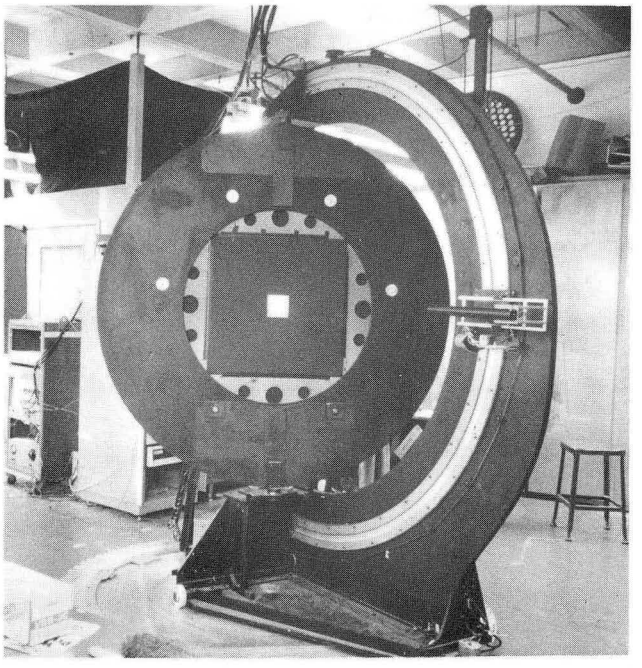


Figure 6. Scanning radiometer for measuring the bidirectional transmittance and reflectance of fenestration components and systems. (BBC 887-6823)

SUPERLITE capabilities to model more sophisticated daylighting systems such as complex sun control and shading systems. This work includes developing and upgrading modeling algorithms and initial efforts to create a photometric data base containing the complex optical properties of shading systems required by SUPERLITE. (Related work on the measurement of these properties is discussed in the earlier section titled "Daylight and Solar Heat Gain Studies.")

We also plan to develop tools to assist designers in qualitative assessment of daylighted environments by using the numerical output of the SUPERLITE program to produce luminance maps of light distributions in architectural spaces.

In FY89 we will provide an initial library of shading system optical properties for SUPERLITE using data from our luminance scanner. Further collaborative work with other university-based groups will be directed toward improving the ease of use of the microcomputer version of the program and enhancing its input/output capabilities.

The Sky Simulator and Daylight Photometric Laboratory

Scale-model photometry is a powerful tool for daylighting design and analysis. Our 24-ft-diameter hemispherical sky simulator (Fig. 7), located on the University of California's Berkeley campus, simulates the effects of uniform, overcast, and clear skies. Sky luminance distributions are reproduced on the underside of the hemisphere; light levels are then measured in a scale-model

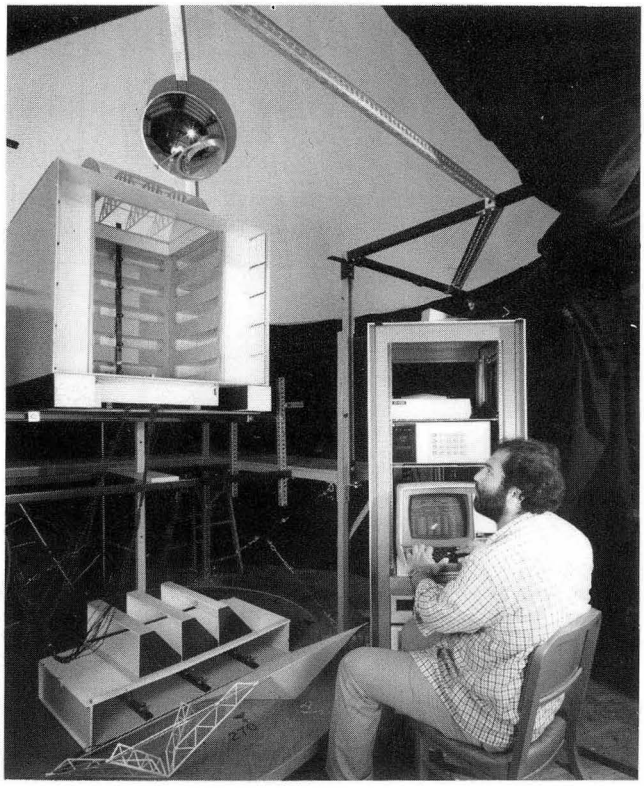


Figure 7. Interior of sky simulator shows reconfigurable scale model of a five-story atrium (with one side of model removed). (CBB 848-5926)

building at the center of the simulator. From these measurements, we can accurately and reproducibly predict daylighting illuminance patterns in real buildings and thereby facilitate the design of energy-efficient buildings. The facility is used for research, for educational purposes, and on a limited basis by architects working on innovative daylighting designs.

FIELD MEASUREMENT OF FENESTRATION THERMAL PERFORMANCE

We have known for some time that winter solar heat gain through south-facing windows in conventional buildings is a significant source of "free" energy. Subsequent calculations have indicated that it is technically possible, for any orientation in any U.S. climate, to optimize windows to the point that they become positive contributors to a building's energy needs.

This claim is not likely to be widely accepted without firm experimental verification. However, to measure the performance of highly optimized window systems in a realistic way is a formidable measurement task, requiring specialized non-steady-state calorimetry on a scale never previously attempted.

To perform these measurements, the Mobile Window Thermal Test Facility (MoWiTT) was designed, built and calibrated. In developing this facility (Fig. 8), it was necessary to solve the problem of doing calorimetry on a

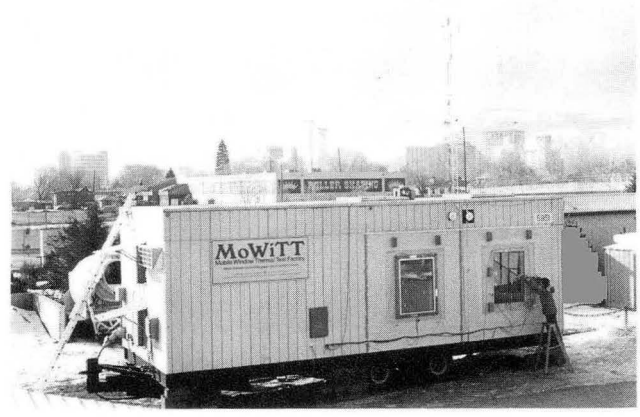


Figure 8. The MoWiTT facility at its field test site in Reno, Nevada. Two sealed insulating glass units are mounted in the two calorimeters. Portable building at left contains computer that controls the facility and records data, including data from on-site weather tower. (CBB 892-812)

room-sized enclosure (which would normally require careful maintenance of constant equilibrium conditions) in the presence of the solar fluxes and changing outdoor temperatures which control the behavior of a fenestration system. We solved this problem with a large-area heat flux sensor (developed as part of the project) and a very sophisticated measurement of the heat extracted from the calorimeter by its cooling system. The MoWiTT began operation in 1986 at a field-test site in Reno, Nevada.

During FY88 we completed a study of windows with frames (a cooperative study with support from the Bonneville Power Administration), which demonstrated that calculated U-values agree well with field measurements, provided that there is adequate knowledge of the local weather conditions. In most cases, results were also consistent with laboratory measurements of U-value; however, laboratory measurements appeared to be questionable for highly conductive frames. This study provides the first convincing evidence that U-value calculations can accurately predict field performance, a question which has been the subject of controversy for more than a decade. The study also demonstrated that the diffuse solar heat gain admitted by north-facing or shaded windows has a significant effect on the daily winter energy balance. This heat gain is frequently neglected in estimates of winter heat loss.

We have also begun measurements of solar heat gain and the inward flowing fraction of absorbed solar energy for windows with shading systems. These measurements form part of the cooperative study of solar heat gain undertaken with partial support from ASHRAE and described above (see Daylight and Solar Heat Gain Studies).

In 1989 we will extend our studies to include higher-performance windows and superwindows, continue the solar heat gain study, and explore the effect of common

shading systems on winter energy performance. We will utilize our data in support of a joint US/Canadian project to standardize the calculation of window U-values.

These measurements with the MoWiTT have the potential for removing uncertainties about window performance that have slowed progress in energy conservation for the past decade.

BUILDING APPLICATIONS AND DESIGN TOOLS

The development of new glazing materials and experimental characterization of fenestration system performance must be complemented by translating the benefits of such information to the building design community. The objective of our building applications activities is to apply the knowledge gained from our basic science research to real-world buildings and develop the tools to disseminate this information.

SIMULATION STUDIES: NONRESIDENTIAL BUILDINGS

Our goal is to develop a microcomputer-based fenestration performance design tool. The first phase of the project, supported by a contract from the Lighting Research Institute and DOE, has been to define a methodology for evaluating overall fenestration performance and construct a data base for conventional fenestration systems and complex operable shading systems. The second phase entails the development of the actual design tool.

A large part of our effort was directed toward reporting the results of Phase 1. In addition to completing the final report, "Commercial Building Fenestration Performance Indices Project, Phase 1: Development of Methodology," we presented a second paper, "An Approach for Evaluating the Thermal Comfort Effects of Nonresidential Building Fenestration Systems," at a comfort symposium and explained the methodology used to define comfort indices. A third paper, "An Indices Approach for Evaluating the Performance of Fenestration Systems in Nonresidential Buildings," describes the overall methodology and was presented at an ASHRAE technical conference.

We began development of the microcomputer-based design tool with special emphasis being placed on the design of the user interface. Of particular importance was our study of the combination of text and graphics that are necessary to give potential users an intuitive sense of the tool's purpose and use. We also implemented several of the algorithms derived during the analytical phase of the project. Figure 9 shows an output screen from this prototype tool. Menu items are shown along the left hand side and the bar diagrams represent calculated values for four fenestration systems.

In FY89 we will to continue our Phase 2 efforts to develop a microcomputer-based tool with co-support from LRI and DOE. The tool will allow a user to access and process the glazing and shading-systems data base to determine the key performance indices as indicated in Figure 9. Simultaneous treatment of the thermal and visual comfort effects in parallel with the energy-related performance data is a major advance over past energy models.

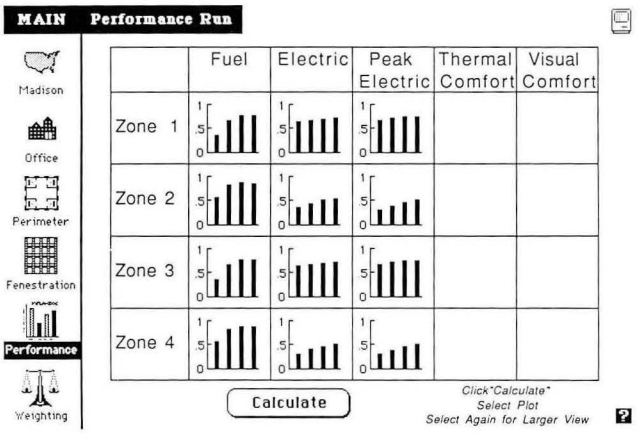


Figure 9. Screen from fenestration design tool shows calculated values of fuel use for heating, electricity use for cooling, and peak electricity demand for four different fenestration systems. (XBL 892-645)

The tool will allow the user to weight each index to find the fenestration system that optimizes energy, cost, and comfort issues based on the user's weighting factors. The tool can also be used directly in an "optimization mode". Since the performance data are stored in simple analytical form, the user can directly determine properties of a real or hypothetical fenestration system representing an optimal solution, i.e., minimum or maximum value for each performance parameter. Combining these analytical capabilities with a hypermedia user interface will produce a powerful and effective design tool. Final design of the overall tool will be based on extensive consultation and testing by project sponsors and feedback from professional user groups.

SIMULATION STUDIES: RESIDENTIAL BUILDINGS

Our objective is to provide home builders and others involved in residential design and construction with easy access to relevant results of our window performance studies. The proliferation of new window technology offers new options to builders, but at the same time the multiplicity of options creates confusion regarding optimal selections to meet all performance requirements. We prepared a draft set of "Window Notes" that define and summarize performance factors for existing and new window technologies that affect residential energy use and comfort. This information was reviewed by the National Association of Home Builders.

Simultaneously with the development of the paper version, we created an interactive computerized version of the notes that included a variety of animation features. Figure 10 shows the main menu of this tool. The highlighted items are those aspects that were completed.

In FY 89 we will begin to expand "Window Notes" into a more comprehensive residential fenestration design manual/tool. This will ultimately include the development of a microcomputer-based simplified analysis tool.

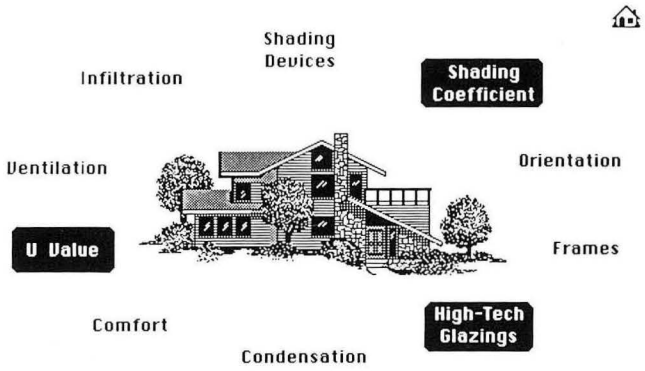


Figure 10. Main menu screen of computerized version of "Window Notes," which summarizes performance factors of window technologies. "Window Notes" will be expanded into a comprehensive residential fenestration design tool. (XBL 892-644)

DESIGN TOOLS AND TECHNOLOGY TRANSFER

To influence energy consumption trends in the United States, it is critical to communicate our results to other researchers and building industry professionals. We use a variety of conventional media to reach a widely varied audience: other research and development groups, educational institutions, design professionals and industrial firms. We continue to develop improved fenestration analysis and design tools and handbooks, carry out design assistance studies, and sponsor workshops and meetings with manufacturing and design firms and public utilities.

Of special significance over the past several years are our efforts to explore new forms of advanced electronic media to better communicate appropriate information to varied audiences. For example, the growing public and private use of CD-ROM (compact disc read-only memory) for storing thousands of pages of text, images and audio reinforces our view of the value to the building community of the technology transfer tools based on new electronic and optical media.

We continued our interactions with the Daylighting Network of North America (DNNA), a group of 35 universities with research and instructional interests in daylighting. The network continued to publish the DNNA News and distribute software packages to faculty and practitioners. The latest advances in the development of "Hypermedia and Future Design Tools" were explored by architectural faculty representing 15 member schools of the network during a Daylighting Summer Retreat in Berkeley. A prototype workstation linking a CD-ROM drive and video disc player with high-resolution color monitor was used to demonstrate the hypermedia-based Daylighting Design Guide prototype we are developing. We expect to involve DNNA members in future development of this tool.

Our research and communication efforts are enhanced by the participation of visiting researchers from the U.S. and including foreign faculty representing Switzerland, Germany, Japan, and Israel. The international perspective provided by our visitors is useful at a time when energy, economic, and environmental issues are increasingly viewed as global concerns.

ADVANCED DESIGN TOOLS

Our long standing interest in developing the next generation of sophisticated hardware and software design tools received significant funding from DOE, allowing us to pursue several exciting avenues. The Advanced Design and Operation Technologies (ADOT) Planning Project is intended to address the development of the technological basis for a family of design tools to be used by designers to achieve greater energy and cost savings in the next generation of U.S. buildings. Private-sector design tools utilizing ADOT technology would contain knowledge bases of energy-efficient technologies and methodologies, computer-aided-design capabilities, energy-analysis modules, and capabilities for visualizing interior and exterior building environments. Visualization capabilities include the ability to realistically simulate both quantitative and qualitative aspects of the building. The interface between the designer and the ADOT tools would rely heavily on visual representations of information and data.

In collaboration with the ADOT Planning Project, we studied imaging and visualization technologies to identify and evaluate the hardware and software requirements for the generation, manipulation and display of visual data for these advanced tools. To demonstrate the potential for the use of dynamic visual information for design decision making and education, we developed a prototype Daylighting Design Guide using new computer-based hypermedia approaches. The prototype is composed of Apple's Macintosh hardware and Hypercard software linked to a CD-ROM drive and video disc player with high-resolution color monitor. The primary thrust of this research is to explore the value and limitations of a hypermedia presentation of traditional daylighting design materials.

We expect to develop a prototype hypermedia information kiosk for demonstration and evaluation purposes with the support of DOE, LBL, and utilities.

PUBLICATIONS

1. Arasteh D, Johnson R, Selkowitz S. Definition and use of a daylight coolness index. Presented at the 1986 International Daylighting Conference, 5-7 November 1986, Long Beach, CA and to be published in the *1986 International Daylighting Conference Proceedings II*, 1989.
2. Benton C, Papamichael K, Arasteh D, Selkowitz S, Spear J. Optical analysis of tracking skylight: soluminaire. LBL-26280, 1987.
3. Johnson K, Selkowitz S. Light guide design principles. Presented at the 1986 International Daylighting Conference, 5-7 November 1986, Long Beach, CA, and to be published in the *1986 International Daylighting Conference Proceedings II*, 1989.

4. Klems J H. U-values, solar heat gain, and thermal performance: recent studies using the MoWiTT. To be presented at the ASHRAE Winter Meeting, Fenestration U-Value Symposium, Jan 29-Feb. 1, 1989, Chicago, IL, and published in *ASHRAE Transactions*. 1988; 95 (Pt. 1), LBL-25487.
5. Klems J H, Keller H. In-situ measurements of u-values and overall thermal performance of windows, LBL-24763, 1988.
6. Kim J, Papamichael K, Selkowitz S, Spitzglas M, Modest M. Determining daylight illuminance in rooms having complex fenestration systems. Presented at the 1986 International Daylighting Conference, 5-7 November 1986, Long Beach, CA, and to be published in the *1986 International Daylighting Conference Proceedings II*, 1989.
7. Kim J, Papamichael K, Selkowitz S. Development of regression equations for a daylighting coefficient-of-utilization model. Presented at the 1986 International Daylighting Conference, 5-7 November 1986, Long Beach, CA, and to be published in the *1986 International Daylighting Conference Proceedings II*, 1989.
8. Papamichael K, Klems J, Selkowitz S. Determination and application of bidirectional solar-optical properties of fenestration systems. Proceedings of the 13th National Passive Solar Conference, June 19-24, 1988, Massachusetts Institute of Technology.
9. Papamichael K, Selkowitz S. Simulating the luminous and thermal performance of fenestration systems. *Lighting Design & Application*, pp. 37-45, 1987.
10. Pennisi A, Lampert C. Optical properties of electrochromic nickel oxide devices utilizing a polymeric electrolyte. Presented at the International Congress on Optical Science and Engineering, Sept 19-23, 1988, Hamburg, FDR. *Proceedings of the Conference on Optical Materials Technology for Energy Efficiency and Solar Energy Conversion VII*, Vol. 1016.
11. Reilly S, Arasteh D. A computer tool for analyzing window thermal performance. Proceedings of the 13th National Passive Solar Conference, June 19-24, 1988, Massachusetts Institute of Technology.
12. Selkowitz S, Papamichael K, Wilde M. A concept for an advanced computer-based building envelope design tool. *1986 International Daylighting Conference Proceedings I*, pp. 496-502, 1987.
13. Sullivan R, et al. An indices approach for evaluating the performance of fenestration systems in nonresidential buildings. *ASHRAE Trans.*, 1987; 94, Pt 2. LBL-23581.
14. Sullivan, R., Arasteh D, Papamichael K, Selkowitz S. An approach for evaluating the thermal comfort effects of nonresidential buildings fenestration systems. Presented at the International Symposium on Advanced Comfort Systems for the Work Environment, Troy, NY, May-1-3, 1988 and to be published in the proceedings.
15. Warren M, Selkowitz S, Morse O, Benton C, Jewell J E. Lighting system performance in an innovative daylighted structure: an instrumented study. *1986 International Daylighting Conference Proceedings I*, pp. 215-221, 1987.
16. Wruck D, Rubin M, Sputtered Electrochromic V_2O_5 Films. *Thin Films*, (in press, 1989).

Lighting Systems Research*

S.M. Berman, R.R. Verderber, R.D. Clear, D. Crawford, D.D. Hollister, D.J. Levy, O.C. Morse, F.M. Rubinstein, M.J. Siminovitch, G.J. Ward, and R. Whiteman

New, efficient technologies and strategies have the potential to save our nation 50% of the electrical energy consumed by lighting, or about 12% of total electrical energy sales. This would amount to a yearly savings of some 220 billion kilowatt-hours of electricity, valued today at more than 16 billion dollars. The significance of this savings can be appreciated by considering projections of economic growth that predict a doubling of present commercial floor space by the year 2020. The 220 billion kilowatt-hours of saved energy would allow the new space to have its desired lighting conditions without the need for new electrical generating capacity, thereby providing an additional capital savings of more than $100 billion.

To help achieve this more energy efficient economy, the Office of Buildings and Community Systems of the U.S. Department of Energy has established a program combining research activities and technology transfer to the lighting community (manufacturers, designers, and users). This program represents a unique partnership between a national laboratory-university complex and industry, facilitating technical advances, strengthening industrial capability, and providing designers and the public with needed information.

Past successes from this effort include development of the high-frequency solid-state ballast for improving the efficiency of fluorescent lamps; the Controlite computer program that enables designers to determine the energy and economic benefits of lighting controls in the workplace; assistance in developing the compact fluorescent lamp; important information on how lighting can effect productivity and visual functions; and determination that both photopic and scotopic spectrum affect the vision process at typical interior light levels.

The program is now actively pursuing development of more efficient light sources through technical concepts such as using isotopically enriched mercury for fluorescent

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Equipment Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF000098.

lamps. A variety of ingenious methods for operating lamps at high frequency without electrodes are being pursued, with the goal of improved efficiency and longevity. In addition, the program is developing comprehensive strategies to optimize the benefits obtained by introducing efficient fixtures combined with lighting controls. This effort is assisted by the use of computers that can display realistic, visual simulation of the lighted workplace. In its study of the relation between lighting variables and visual function, the program is identifying human responses to lighting conditions, leading to new innovative products that improve both energy efficiency and productivity.

The program has identified new long-range technical concepts which, although high in risk, have great potential payoff. These include development of more efficient fluorescent lamp phosphors, lamps filled with novel gases, super fixture systems that overcome the inefficiencies associated with overheating, as well as the use of the spectral quality of lighting to optimize performance and comfort.

This interdisciplinary program encourages innovation in the industry, accelerates the societal benefits obtainable from a more cost-effective and efficient lighting economy. Because of its comprehensiveness, it is unique in the United States.

Since its inception in 1976, the LBL Lighting Program has produced more than 124 reports and publications. These reports, available to the public, document research on subjects such as solid-state ballasts, operation of gas-discharge lamps at high-frequency, isotopically enriched fluorescent lamps, energy-efficient fixtures, lighting control systems, and visibility and human productivity. In addition to its research activities, the internationally recognized interdisciplinary staff is involved in a variety of professional, technical, and governmental activities.

The Lighting Program combines the facilities and staff of LBL with those of the University of California College of Environmental Design and School of Optometry, both on the Berkeley campus, and the School of Medicine in San Francisco (UCSF).

Described below are highlights of the accomplishments realized in FY 1988 by each of our three major efforts: advanced light sources, building applications, and health impacts. Discussion of activities planned for FY 1989 are included in the highlight descriptions. Publications and conference presentations from the past year may be found at the end of this chapter.

ADVANCED LIGHT SOURCES

The advanced light sources effort promotes new lamp technology and light source development. To see what can be accomplished in this area, consider that the most efficacious four-foot fluorescent lamp, operated at high frequency (20 kHz), has a luminous efficacy of approximately 100 lumens of light output per watt of electrical power input. Although this is more than five times as efficient as an incandescent lamp, still greater efficacies are possible. White light can, theoretically, be produced at almost 350 lumens per watt. The advanced lamp technology program is developing the engineering science that will help us achieve a target efficacy of 200 lumens per watt within the next few years.

In the area of fluorescent lamps, three loss mechanisms are candidates for efficiency improvements. These are self-absorption of ultraviolet (UV) radiation, electrode losses, and energy loss in lamp phosphors. In the first case, we would like to reduce self-absorption of UV radiation, a process that occurs within the lamp plasma before the radiation strikes the phosphor-covered inner wall (the phosphor converts UV radiation into visible light). If UV self-absorption is decreased, thereby reducing the chance of quenching electron collisions, the amount of UV radiation available to be converted into light at the lamp wall is increased.

In the second case, energy losses associated with electrodes can be eliminated by exciting the lamp plasma at radio frequencies (RF). The problem is to find an efficient method for coupling the RF energy into the lamp without causing new losses.

In the third case, we would like to develop a more efficient phosphor matrix that will convert one energetic UV photon into two visible photons. These concepts could lead to significant improvements in lamp efficacy.

LBL is studying several ways of reducing UV self-absorption. The first method is altering the isotopic composition of mercury. In its natural state, mercury has seven stable isotopes, each with slightly different resonance UV emission spectra. Altering the naturally occurring isotopic composition can provide more escape channels for the resonance radiation, thereby reducing the probability of quenching collisions and increasing the amount of UV radiation reaching the phosphor. The most promising possibility is isotope alteration-enrichment with ^{196}Hg, which is being pursued in a joint effort by LBL and GTE Lighting. Should isotopic alterations prove economical, modified lamps would enter the market quickly. Lamps would simply be loaded with isotopically enriched rather than natural mercury, with other lamp manufacturing processes remaining the same.

Another method of reducing UV self-absorption was recently discovered at LBL based on the application of a d.c. magnetic field having a direction parallel to the main current. Axial magnetic field strengths of about 600 gauss can increase light emission by about six percent. LBL and major firms in the lamp industry are studying practical ways to apply this technique.

A highly promising mechanism developed at LBL uses a plasma coupling principle that eliminates the need for electrodes; it allows lamp plasma excitation to occur primarily near the inner lamp wall, thereby reducing both the electrode loss and the likelihood of entrapment loss. This surface wave mode of operation occurs at high frequencies in the RF range between 100 and 500 MHz, permitting efficient lamp excitation without electrodes. The surface wave fluorescent lamp shows approximately 40 percent increased energy efficacy over normal fluorescent lamps, operates without starting circuits, and should be very long-lasting because of the absence of electrodes.

Reducing the effects of energy loss in the phosphors requires alteration of a lamp's phosphor material. The

materials used today convert each UV photon into, at most, one visible photon. Improving this conversion rate would increase the efficacy of low-pressure discharge lamps. Although a UV photon has sufficient energy to permit conversion of the UV photon into two visible photons, this process must occur quickly to prevent heat-producing collisions. LBL and GTE lighting are examining the possibilities of a program in phosphor chemistry designed to discover whether the two-photon phosphor is feasible. The lamp industry, long aware of the complexity of this problem and the extensive research required to provide solutions, is extremely interested in this cooperative effort.

If these research projects at LBL come to technological and commercial fruition, future fluorescent lamps would operate at high frequency without electrodes and would be isotopically enriched, magnetically loaded, and coated with a two-photon phosphor. Such lamps would have an efficacy of more than 200 lumens per watt, doubling the efficiency of today's best fluorescent lamps.

Other lamp technology research concentrates on high-intensity discharge (HID) lamps, which could be made both more efficient and dimmable if operated without electrodes. High-frequency operation is required to excite the lamp plasma in an electrodeless mode; it may also permit lamps to function with just one or two metal halides and no mercury or sodium. Electrodeless operation would also enable us to use compounds that have desirable light output and color, but that are excluded today because they would harm electrodes. Finally, an electrodeless lamp that could be dimmed without observable spectral changes and that could provide instant restrike could be used in many new ways. It would improve energy efficiency and would be aesthetically attractive enough for widespread use by lighting designers.

Mercury Isotope Separation and Enrichment of Fluorescent Lamps

Continued progress has been made in assessing the feasibility of photochemical separation of natural mercury to produce mercury enriched in the isotope mass ^{196}Hg. Most of the FY 1988 effort has been involved in designing and building a scaled-up reactor that can produce several grams per day of enriched mercury. This has required the development of a high flux light source now in place. Several new scientific and technical personnel have been added to the project, and a number of new developments are expected in FY 1989. These include in situ measurement of reactor performance, allowing continuous monitoring, production of enough enriched mercury to permit a high speed dispensing procedure (suitable for filling a large number of lamps with the enriched product), and economic analyses of the complete photochemical process that will permit conclusions on the feasibility of enriched mercury lamps as a market product.

Surface Wave Lamp (SWL)

Two important new findings were made during FY 1988. First, the surface wave mode of coupling was extended into a much higher power range, achieving about 10 watts per inch of discharge (as compared to the previous loading of about 1 watt per inch, typical of today's fluorescent lamps). This new level is still an order of magnitude below the 100 watts per inch typical of commercial high intensity (HID) lamps. The intermediate level achieved, which we refer to as the MID lamp, still maintains the zero reflected power condition essential for achieving high efficacy. A noteworthy aspect of the MID surface wave lamp is its instant restrike capability compared to the typical 10-minute period needed for commercial HID lamps. The question of effective coupling and restrike capabilities at an HID condition will be considered during the next year.

Our second major achievement is the development of a launcher and the finding of a frequency that allows a two-foot lamp to be energized by the surface wave mode. Efficacy improvements of about 30% for the longer-length lamp have been achieved.

Our first written examination of possible SWL power supplies indicates that a Class E amplifier with a solid state switching transistor is the most likely candidate. Further work in FY 1989 in this area will be undertaken with an outside contractor familiar with Class E amplifiers.

Electrodeless High-Intensity Discharge (HID) Lamp

The complete system for back-filling lamps 1 in. and .75 in. in diameter has been completed. These lamps are spherical in shape and are to be filled with various candidate materials for efficient HID light production. Successful glow-to-arc transition has been obtained with a pure mercury fill at slightly over 100 watts of lamp power.

Knowledge of the actual pressures in the lamp at operating conditions will be absolutely essential. For this purpose, several techniques have been initiated. The potentially best method involves insertion of a small amount of scandium (about 1% by mass) into the lamp. Scandium has some optically thin emission spectra in the visible region, and these line widths can be measured quite accurately. These scandium lines have been observed, and the success of this method will depend on an accurate calibration procedure which will be developed during FY 1989.

Lamp Fabrication Facility

Much effort in FY 1988 has been expended on developing our own lamp fabrication facility, which will enable us to build lamps from the basic glass tubing, fill with the desired gases and salts, include glass electrode seal if needed, and use all the extensive combined vacuum and oven systems needed for fill control and maintenance

of high purity. The facility required a new laboratory room that was constructed by conversion of a large, partially open storage area. Our personnel designed the facility and monitored its rehabilitation. The various fabrication components were tested and incorporated into the integrated facility. Numerous difficulties were encountered because of scheduling delays brought about by overall LBL plant complications; nevertheless, the lamp facility achieved 90% completion by the end of FY88, with the 100% level expected in early FY 1989 (Figures 1 and 2).

Isotope Modeling

This project, a joint effort with New York University, has the primary objective of developing a theoretical model to account for the effects of variations in isotopic mercury composition upon emittance of a low-pressure discharge. The secondary objective is to include the effects of partial redistribution, surface effects, and line-shape factors that affect the emittance, and hence the efficacy, of UV radiation.

The practical goal is to specify the isotope composition that maximizes emittance.

Figure 1. Evacuated glove box where hydroscopic salts are prepared as additives for lighting producing fills in electrodeless HID lamps (CBB 876-10627)

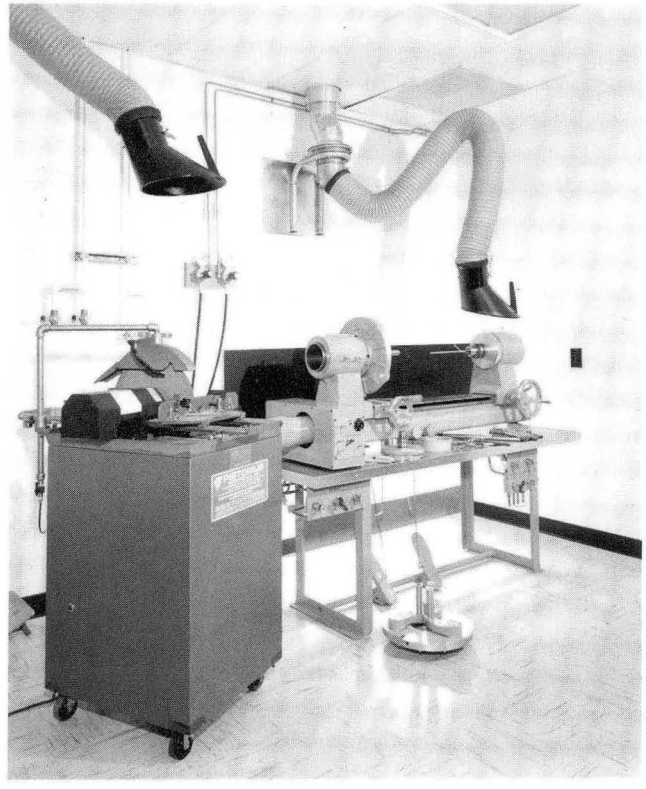


Figure 2. Lamp fabrication components including glass lathe (right) and high-speed glass saw (left). (CBB 891-341)

We have formulated a variational theoretical model of the radiant emittance of the mercury-argon discharge used in fluorescent lighting. The model includes the effects of the fine structure and isotope shifts in the resonance radiation line as well as those of atomic diffusion, resonant exchange of excitation, and radiation transport. The result is a variational principle which, when evaluated using suitable trial functions, yields a variational estimate of the radiant emittance of the discharge. This principle is used to study the effects of isotopic mercury enrichment on emittance. The special case of a single pure isotope, as well as mixtures of all seven naturally occurring isotopes, are presented. Recent experiments with enhanced ^{196}Hg and ^{201}Hg concentrations are discussed within the context of this theory. The relative merits of three isotopic mixtures recently proposed for commercial development by Alchemie, Inc. are assessed, and one of the mixtures (case 2) can be expected to lead to a greater improvement of the emittance of the discharge than the other two, with about a four percent increase over that of natural Hg. Further refinements, including additional physical effects as well as improved numerical codes, are planned for the final stage of the model.

BUILDING APPLICATIONS

Real energy savings depend on the transfer of energy-efficient technologies and strategies to the lighting

community. The building applications activities aim to assess and develop energy-efficient lighting technologies and to combine their technical performance characteristics to model energy-efficient and cost-effective lighting geometries and controls. Our analysis uses knowledge of the relationship between visual performance and physical aspects of lighting, such as illumination level, distribution, contrast, and glare. As part of this effort, a computer program has been developed that provides accurate simulations of illuminated spaces with their contents. The simulated scenes are visibly indistinguishable from real photographs; using them, we can model effects of changes in the illumination systems. Validation of luminance values produced by these simulations requires physical measurements of luminances in complex environments. Therefore, the project uses a number of novel techniques for real luminance mapping of interior environments with complex objects to obtain actual luminance values. The technology development component of this program examines engineering approaches to reducing light losses associated with thermal factors of conventional lighting fixtures. The conclusion of these efforts will be a combination of lighting systems technologies and analysis. Visual simulation of the proposed application represents the most compelling tool for promoting the implementation of energy efficient lighting.

Advanced Lighting Design

The primary objective of this effort is the development of simplified guidelines for assessing lighting contrasts, and hence, performance available in a given space as a result of illumination, fixture geometry, lamp type, and interior reflectance. The procedures involve examination and analysis of available computer programs.

During FY 1988, parametric runs on Lumen-Micro were studied to examine the question of the effect of luminaire spacing and the light distribution from particular luminaires on predicted visual performance in an open-office environment. Optimal spacing geometries have been determined. A cost-benefit analyses will be undertaken during FY 1989, taking into account the tradeoffs between higher light levels and tighter spacing with potentially diminishing returns on productivity.

Energy-Efficient Luminaires and Thermal Control Devices

Ceiling-mounted four-lamp luminaires, lens and parabolic types, were evaluated during FY 1988. The minimum lamp wall temperature of the in-place lamps were measured with various ventilation schemes and distances from the ceiling. Simple convective cooling reduced the excessive lamp wall temperature 10° to 15°C and was a function of distance from the ceiling. The thermal performance of the luminaires was measured for standard ballasts with 40-watt and 34-watt lamps, and for electronic high-frequency ballasts. The convective cooling strategy was able to recover most of the thermal loss due to lamp overheating.

During FY 1989, the thermal performance of enclosed and parabolic four- and two-lamp troffers will be measured. We will also develop optimum venting to convectively cool the fluorescent lamps controlling the ambient and plenum temperature. Measurements using a standard two-lamp F40 lamp-ballast system will be conducted for reference and compared with measurements for energy-saving magnetic ballasts and electronic ballasts.

In the area of specific devices to control lamp wall temperature, our major effort has been on concepts that use the Peltier effect coupled with a heat pipe acting as the heat sinking component.

The power to the Peltier device was obtained from the secondary filament windings of a standard ballast. This was accomplished by a filtered full wave rectifying circuit. The capacitor required is relatively large; operating the Peltier device from an unfiltered source would have a practical advantage.

An experimental variable conducting heat pipe was designed and constructed. This elegant concept requires no external power source to control lamp wall temperature.

An experimental test station constructed to evaluate the performance of these devices was used to measure the lamp-ballast combination (Figure 3).

A number of important questions regarding the efficiency of heat transfer will be examined during FY 1989. In addition, a study of the limitations of using rectified AC power (instead of DC power) for Peltier devices will be carried out. If the devices can be operated by half-wave or full-wave rectified power, the DC conversion costs could be greatly reduced.

Quality Illumination and Performance

During FY 1988, we completed an analysis of our 17-subject study of the speed of reading unrelated words. The time to read these words was measured with an

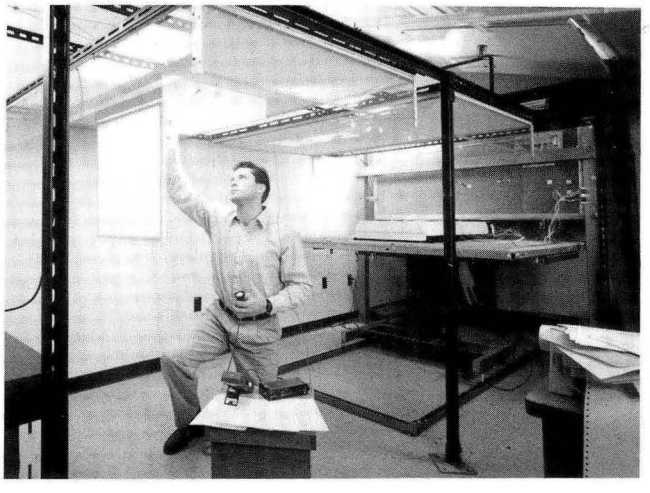


Figure 3. Luminaire laboratory with heat pipe being installed on fluorescent lamp. (CBB 89-345)

eyetracker that could determine fixation time as well as the time for a saccade. The contrast, luminance, and size of the words was controlled and varied over ranges typical of office work. The analysis showed the remarkable result that the reading speed data could be solely a function of the ratio of letter size to threshold size; the dependence on contrast and luminance occurs only through their effect on threshold size. The results indicate that a useful and simple field test can be made available to determine if a given individual has adequate illumination (or contrast) for any given reading task.

The work is currently being prepared for journal publication and for the 1989 annual meeting of the Illuminating Engineering Society.

Additional efforts on improved cost-benefit techniques have been pursued. A new model of basic visual performance shows promise of overcoming the criticisms leveled at the models by Rea and by Blackwell.

Computer Imaging

The RADIANCE modeling system was ported to the SUN workstation in FY 1988. "Alpha" test versions of the RADIANCE program were released to selected faculty and students at UCB Schools of Architecture and Optometry and to the University of Michigan Architecture Department to solicit comments and feedback from users. In 1988, RADIANCE was validated against Superlite and against daylit scale models composed of diffusely reflecting surfaces. Further validation needs to be carried out with physical measurements of specular and semi-specular materials under artificial light. A three-dimensional editor has been developed on the Macintosh and was ported to the X-windowing system on the SUN workstation. Additional utilities to improve program usability were also added.

Effort in 1989 will be devoted to completing the verification of RADIANCE accuracy by comparing calculations with empirical measurements from both scale and full-size models.

In addition, a lighting design firm will be selected to work with LBL, using RADIANCE software to design a complete energy-efficient lighting system.

IMPACTS OF NEW LIGHTING TECHNIQUES ON PRODUCTIVITY AND HEALTH

The idea that lighting might negatively affect health has appeared often in the lay press during the past few years. Scientific data are lacking, especially to ascertain whether new energy-efficient technologies adversely affect human health and productivity.

Performance and productivity may be influenced by lamp electronics and associated controls, fixtures, or the geometry and location of the lighting system. We classify these lighting factors as color variations; glare; intensity fluctuations; spectrum variations, including the ultraviolet region; electromagnetic fields generated by the lamp, ballast, or controls; and flicker. All of these could evoke a variety of human responses (behavioral, psychophysical, physiological, or biochemical).

Our research seeks to assure that new energy-efficient lighting technologies do not adversely affect human health and productivity. We are investigating whether any aspect of new technologies can produce responses in humans. If we identify responses, we will characterize the effects and identify the necessary changes in lighting technologies. Although subjective responses of workers provide some information, such responses are generally confounded by a mix of sociological factors and individual motivations. The investigations carried out by LBL use objective responses to establish cause and effect, and ensure repeatability.

The impacts program is divided into two areas: 1) direct effects of lighting on the human autonomic system (carried out at University of California, San Francisco and LBL); and 2) interactions of lighting that affect visual performance and productivity or comfort (carried out at the UC School of Optometry and LBL), which are termed here "lighting ergonomics."

In the first area of this program, lamps to be evaluated include incandescent, cool-white fluorescent, high-pressure sodium, and metal halide. Human responses to various lighting conditions will be assessed by monitoring autonomic responses including heart rate, galvanic skin response, muscle strength, exercise tolerance, facial expression, and pupillary response. Behavior measures to be used include memory (Wechsler Memory Scale and Sternberg's Memory Scanning Time), cognitive function (mental arithmetic), time estimation, and simple reaction time. Other behavioral tasks will probably be included.

Data gathering and subject control are supervised by trained medical personnel. A national technical advisory committee oversees and reviews the project. First results of this effort concern the effects of visible spectrum and low-frequency radiation on human muscle strength and, as described previously, they indicate that psychological factors are the likely cause of reported effects. A second set of experiments using infrared pupillometry has, however, demonstrated that the spectral response of the pupil at typical interior light levels is the scotopic spectrum and thus that red photoreceptors are active at these light levels.

The second area of this program primarily studies issues of glare and flicker resulting from lighting systems.

Present knowledge and prescriptions by the lighting community for dealing with glare are based on subjective responses without support by objective criteria. It is reasonable to implicate pupillary responses as relevant to glare discomfort because pain receptors are present in the iris, and the nervous pathway necessary to signal pain is present in the fifth trigeminal cranial nerve. Some studies by vision scientists have suggested pupillary response as a possible objective correlate to the sensation of discomfort, but this conclusion is not generally accepted in the vision community. We have undertaken a series of studies to

clarify the possibility that pupillary dynamics can be used as an indicator of glare response.

Visual system responses to the oscillating light levels pervasive in our interior environments has also been implicated in many anecdotal reports. The program has undertaken a series of direct physiologic measurements to investigate whether such responses can be established.

Direct Effects of Lighting on the Human Autonomic System

The first phase of work on brightness perception has been completed, clearly demonstrating a significant contribution of scotopic spectrum to brightness as perceived by subjects in a room. This result, coupled with our previous finding showing the scotopic spectral response for pupil size, implies that under typical interior light levels, vision function is mesopic, i.e., both rods and cones of the retina are active. Our present experiments are consistent with a brightness function expressed by the equation $B = \log P + 0.9 \log S$, where B is the perceived brightness while P and S are the values of the viewed photopic and scotopic luminance. The significance for energy efficiency demonstrated by this equation can be seen by comparing warm white and daylight fluorescent lamps of equal wattages, in which case the daylight illuminant will appear twice as bright. The value of 0.9 in the above equation has some uncertainty, and the second phase of this effort (to be accomplished in 1989) will determine more precisely the quantitative mix of photopic and scotopic spectrum that correlates with perceived brightness.

The most compelling demonstration of rod contribution to brightness perception will be shown by the pupil stimulator. This device, under development at LBL, will allow brightness comparisons to be made with periodic time, varying luminances where the oscillation rate can be adjusted to occur below and above the rod fusion frequency. Currently, the instrumentation is undergoing revisions and the system optics are being altered in order to incorporate the new, more intense light sources. These new light sources will allow a much better focusing capability into the fiber optic system that was not very efficient with the previous choice of light source, i.e., the tungsten halogen lamps. The construction is expected to be completed during FY 1989.

The effects of pupil size on visual performance are being studied by observing the contrast sensitivity of subjects. The experimental protocols have been established and the software developed to allow the equal-luminance double grating to appear simultaneously on the TV screen. Subjects will then choose which of the two presentations is the grating, i.e., only one side of the rectangular page projected will actually be a vertical grating (the other will simply be a uniform equal-mean-luminance rectangular patch). Figure 4 shows the chamber at the UCSF laboratory where the pupil measurements are performed.

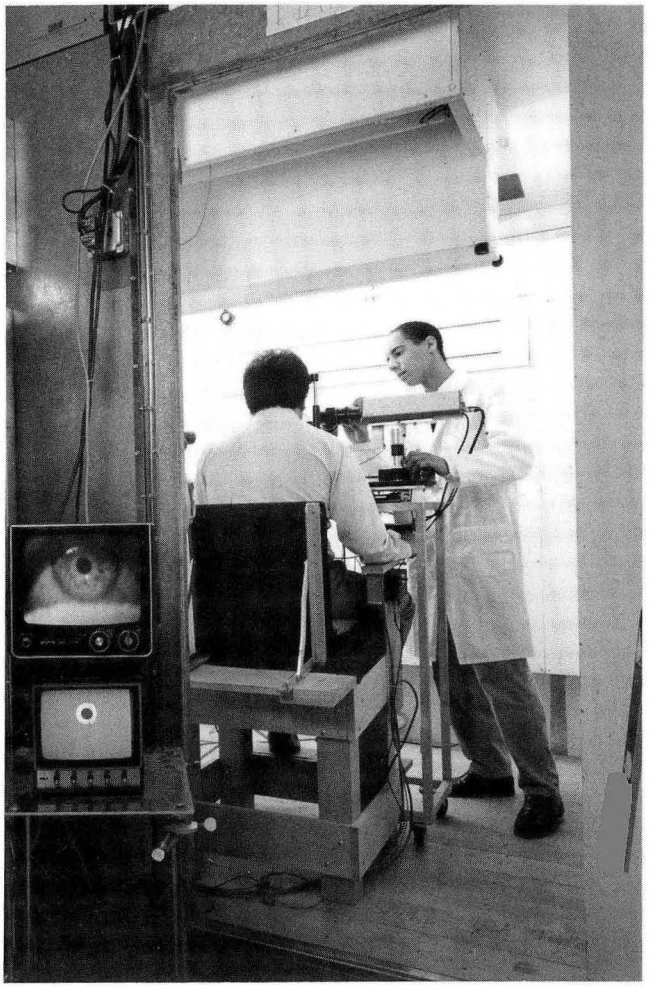


Figure 4. Subject seated in lighting test chamber is being prepared for pupil measurements by remote infrared pupilometry. (CBB 870-10637)

Lighting Ergonomics

Discomfort Glare Studies

We have completed experimentation on the frequency spectrum of pupillary unrest (hippus) under conditions of the absence of discomfort glare and in the presence of discomfort glare where the light levels were set to provide equal mean pupil area. This condition is achieved by producing the pupil size with a bright but large area source while the discomfort glare condition is achieved with a small, intense glare source in a relatively low-level uniform surrounding. The frequency spectrum is then determined by Fourier transform of the time, varying pupillary unrest and the two lighting conditions compared. The results show no observable differences in spectrum shape

or intensity. Our conclusion is therefore contrary to previous results and claims that argue for a difference on the hippus spectrum.

Experiments planned for FY 1989 will test the hypothesis that pupillary response is associated with the sensation of discomfort glare. A pilot study on the influence of color on discomfort glare showed that for small geometric sizes of the glare source, the sensation of discomfort had a definite spectral response, with the more blue or red portions of the spectrum being more efficacious in eliciting the discomfort. This preliminary result is consistent with brightness perception for small sources. This is the first known controlled effort on the spectral response of discomfort glare, and this effort should give lighting designers and users useful information about this form of glare. The effort is anticipated to be completed during FY 1989.

Electroretinogram Studies of Flicker

Microelectrode studies in the cat visual system as well as visual evoked potential and electroretinogram (ERG) studies in humans have demonstrated synchronous responses to periodic time-varying stimuli at frequencies higher than human perceptual fusion. We have determined the time-averaged ERG responses of two human subjects who viewed text on a visual display unit (VDU) at typical values of luminance and contrast. The refresh rate of the VDU was varied in 5 Hz increments between 46 and 81 Hz. In addition, we measured the ERG response in one subject with intense flickering light, provided by a projector and rotating sector disc, to examine whether synchronous ERGs could be obtained at frequencies as high as those found to produce responses in the cat eletrophysiologic studies (100-120 Hz). For the VDU stimulus, we found clearly identifiable synchronous ERG responses at refresh rates as high as 71 Hz. Synchronous responses to the more intense source were clearly evident at frequencies as high as 162 Hz. Figure 5 shows subject with the electroretinogram lens in place.

A further study was initiated to examine whether this subject would show an ERG response when directly viewing a two-lamp fluorescent light fixture. Fluorescent lamps conventionally operate on line frequencies of 50 Hz in Europe and 60 Hz in the United States and provide light output that is modulated and oscillating at twice this line frequency. At these "high" frequencies, any consequencies of "flickering" light level have been presumed to be absent because the oscillation rate is above that perceivable by humans. However, the subject showed a direct physiologic response to fluorescent lamp modulation in terms of synchronous retinal responses in electroretinogram measurements at frequencies even higher than the 120 Hz oscillation rate. Thus, there is some evidence of responses to light oscillation even though they are not directly perceived. Whether such responses could be related to the reported symptoms of headaches and eyestrain remains to be established. The studies are now being prepared for submission for publication in the vision science and lighting literature.

Figure 5. Close-up view of subject with electroretinogram lens inserted into left eye. Lens consists of a circular wire on a contact plastic on the cornea and a silver speculum resting against the sclera. (CBB 876-4387)

PUBLICATIONS

1. Verderber R. Energy efficient lighting on board naval ships – phase II – the T-8 lamp system. 1987 (LBL-23153).
2. Rubinstein F, Verderber R, Ward G. Photo-electric control of daylight following lighting systems (daylight sensing photocell placement). *Electric Power Research Institute*, 1987 (LBL-24872).
3. Berman S, Greenhouse D, Bailey I, Raasch T. Human electroretinogram responses to visual display flicker. *The Association for Research in Vision and Ophthalmology (ARVO) Annual Meeting Abstract Issue*, Vol. 29, May 1-6, 1988, Sarasota, FL (LBL-24666).
4. Rubinstein F, Ward G, Verderber R. Improving the performance of photo-electrically controlled lighting systems. *Proceedings of the IES Annual Conference*, August 7-11, 1988, Minneapolis, MN (LBL-24871).
5. Ward G, Rubinstein F. A new technique for computer simulation of illuminated spaces. *Journal of the IES* 1989; 18(1): 80-91 (LBL-23042).
6. Clear R, Berman S. Estimation of linear interpolation error. *Journal of the IES*, in press, 1988 (LBL-24811).
7. Verderber R, Morse O, Rubinstein F. Performance of electronic ballast and controls with 34- and 40-watt fluorescent lamps. *Proceedings of the IEEE-IAS Annual Conference*, October 1-3, 1988, Minneapolis, MN (LBL-25429).
8. Verderber R, Rubinstein R, Siminovitch M. Control of lamp wall temperature. *Proceedings of the IEEE-IAS Annual Conference*, October 1-3, 1988, Minneapolis, MN (LBL-25430).

INDOOR ENVIRONMENT PROGRAM STAFF

David Grimsrud, Program Leader
Anthony Nero, Deputy Program Leader

Kathleen Alevantis
James Allen
Michael Apte
Stephen Brown
Edie Canfield
Edward Churka
Joan Daisey*
Nancy DeMello
Richard Diamond
Darryl Dickerhoff
Helmut Feustel
William Fisk†
Karina Garbesi
Ted Gartner
Lara Gundel
Jed Harrison
Alfred Hodgson
Nori Hudson
Anne Kovach
Anna Lee
Mark Modera
Nancy Morrison
William Nazaroff
Timothy Nuzum
Denise Odenwalder
Richard Prill
Kenneth Revzan
Alan Robb
Greg San Martin
Gail Schiller
Richard Sextro*
Max Sherman*
Brian Smith
Carol Stoker
Richard Szydlowski
Lucia Tin
Greg Traynor
Bradley Turk
Henrik Wallman

*Group Leader
†Acting Group Leader, 8/88-8/89

INDOOR ENVIRONMENT PROGRAM

INTRODUCTION

The Indoor Environment Program examines the scientific issues associated with the design and operation of buildings to optimize building energy performance and occupant comfort and health. Optimizing occupant health and comfort is addressed in various ways by groups within the Program. To examine energy flow through all elements of the building shell, the Energy Performance of Buildings Group measures air infiltration rates, studies thermal characteristics of structural elements, and develops simplified models of the behavior of complete buildings. Potential savings in the infiltration area are great. The heat load associated with natural infiltration is about 2.5 quads/yr costing about $15 billion annually. It may be economic to reduce this by 25%.

This change, however, may produce undesirable effects in the building environment. Since ventilation is the dominant removal mechanism for building pollutants, concern continues about the impact of designs or changes in operation that lead to its reduction.

This issue has been an important theme for other projects in the Program. Efforts include characterizing the emission of various pollutant classes from their respective sources, studying the effectiveness of ventilation in removing pollutants from indoor atmospheres, and examining the nature and importance of chemical and physical reactions that can affect the production of airborne pollutants. Projects have concentrated on three major pollutant classes: combustion products arising from indoor heaters and other combustion appliances; radon and its progeny, arising from materials (primarily soil) that contain radium, a naturally occurring radionuclide; and formaldehyde and other organics, arising from a variety of building materials and furnishings. In addition, the Ventilation and Indoor Air Quality Control and Energy Performance of Buildings projects investigate techniques for controlling airborne pollutant concentrations, develop devices for monitoring pollutants in laboratories and buildings, and design or carry out field surveys of energy use and indoor air quality in residential and commercial buildings. The Indoor Exposure Assessment project also devotes time to assessing the health effects of indoor pollutant exposures. We continue to explore several important themes:

A. **Air quality in buildings is dominated by sources.** Problems are more often related to strong indoor sources than to deficiencies in ventilation.

B. **Air pollution is a buildings problem.** Pollutants concentrations observed in buildings are comparable to those outdoors (when major indoor sources are present, the concentrations indoor are substantially higher). Since people spend 70-90% of their time inside buildings, the major portion of their exposure to air pollutants occurs within buildings. We conclude that air pollution is a buildings problem because sources and removal processes are often associated with building structure and operation.

C. **Ventilation is the best control strategy for indoor pollution.** Ventilation using outdoor air affects all indoor pollutants similarly and is therefore, the best single strategy for pollutant control in buildings. This assertion acknowledges that we cannot identify all pollutant sources in a building. Since such information is often lacking, ventilation remains the best general indoor pollution control strategy.

Evaluation of Several Techniques to Reduce Radon: Preliminary Results from Fourteen Houses *

B.H. Turk, J. Harrison, R.G. Sextro, L.M. Hubbard†, K.J. Gadsby†, T.G. Matthews‡, C.S. Dudney‡, D.C. Sanchez§

Fourteen homes with basements and hollow block foundation walls in north-central New Jersey, were selected for this research project. Seven homes were studied by Lawrence Berkeley Laboratory, while the other seven were studied by Oak Ridge National Laboratory and Princeton University. One home from each group of seven did not have a radon control system installed, and served as a control

Beginning in the fall of 1986, radon concentrations and other parameters in the homes were intensively monitored with continuous, real-time instrumentation. Monitoring continued for 7 to 13 months. We developed diagnostic procedures to guide choice of the appropriate radon reduction technique in each house. Oak Ridge National Laboratory and Princeton also used a modification of these diagnostic procedures. Radon control systems were designed to: (1) effectively and economically reduce indoor radon concentrations below 148 Bq m^{-3} (4 $pCil^{-1}$), and (2) allow comparison of a variety of mitigation systems. These were installed beginning in November, 1986. System-types included: subsurface ventilation (SSV) by depressurization (SSD), and SSV by pressurization (SSP) in 11 homes, ventilation of perimeter drain tiles/drain ducts (eight homes), air-to-air heat exchangers (AAHX) in two homes, basement pressurization (three homes), block wall ventilation (three homes), and caulking and sealing openings to the soil (all homes).

Subsurface ventilation by depressurization was very often recommended and successful. SSP was less effective than SSD in all homes where it was evaluated. This contrasts with results from earlier studies in the Spokane, WA area. Drawing air from the cores of block walls and SSV via a connection to perimeter drain (perimeter of basement slab floor) were generally effective due to the efficient ventilation and depressurization of major subslab regions from which radon normally entered the house. Pressurization of basements with air drawn from upstairs caused satisfactory reductions in indoor radon levels in only one house where the basement could be sufficiently tightened to permit adequate pressurization. The AAHX's reduced radon concentrations to an extent consistent with the theory that concentrations are proportional to the reciprocal of the total ventilation rate when ventilation is not associated with a change in indoor air pressures. This supports previous work indicating that AAHX's are generally adequate only in homes with low initial indoor radon levels and ventilation rates. Finally, caulking and sealing often resulted in a measurable reduction in baseline indoor levels, but never achieved the target concentration.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division, by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Research Division of the U.S. Department of Energy (DOE) under contract no. DE-AC03-76SF00098, and by by U.S. Environmental Protection Agency (EPA) through Interagency Agreement DW89931876-01-0 with DOE. The work by ORNL/Princeton was co-sponsored by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments and Pollutant Characterization and Safety Research Division of DOE under contract no. DE-AC03-84OR21400, by the EPA through IAG-40-1709-85 with DOE, and by the New Jersey Department of Environmental Protection.

†Princeton University
‡Oak Ridge National Laboratory
§U.S. Environmental Protection Agency

Intensive Radon Mitigation Research: Lessons Learned*

B.H. Turk, R.J. Prill, R.G. Sextro, and J. Harrison†

Two intensive field studies of radon control have provided an opportunity to conduct follow-on research, and to compare and combine data and results from regions with different soils and types of house construction. The first study near Spokane, Washington involved 14 homes often having foundation walls of poured concrete placed in soils of uniformly high permeability and low to moderate soil gas radon concentrations. The second study was conducted in north-central New Jersey on seven homes that had foundation walls constructed of hollow core blocks. The soils around the New Jersey homes were variable in both permeability and radon concentrations in soil gas.

For control homes (homes that did not receive radon control systems until conclusion of the projects) in both studies, indoor radon levels remained higher than expected in the spring and summer. During these seasons, the warmer outdoor air temperatures are expected to diminish the thermally-caused negative pressure differences that drive the bulk flow of radon-containing soil gas into the houses. It was discovered that soil temperatures substantially modify the pressure differentials (ΔPs) that drive soil gas entry into basements in both summer and

*This work was supported by the Bonneville Power Administration (BPA) under contract no. DE-A179-83BP12921, by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division, by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Research Division of the U.S. Department of Energy (DOE) under contract no. DE-AC03-76SF00098, and by the U.S. Environmental Protection Agency (EPA) through Interagency Agreement DW89931876-01-1 with DOE.

†U.S. Environmental Protection Agency

winter. Calculations for a one-story house in New Jersey show that warmer soil in winter and cooler soil in summer (relative to the prevailing outdoor temperatures), reduces the magnitude of the basement pressure difference by about 1 Pa. At times during the summer, the cooler soil gas temperatures can cause the ΔPs to be negative, drawing radon into the building.

Another finding is that the forced-air distribution of many residential heating and cooling systems can increase the natural depressurization of the substructure by up to 10 Pa (but generally less) and also transfer large amounts of radon from the substructure to the upper floors. These effects are more pronounced if leaky return air ducts or plenums are located in the substructure.

For the majority of homes in these two studies, subsurface ventilation (SSV) was the most appropriate and effective radon control technique. The data and measurement results indicate that 40% to 90% of the air in SSV exhaust airstreams originates in basements. This suggests that the leakiness of the below-grade substructure surfaces greatly influences the flow resistance to an SSV system.

Air-to-air heat exchangers (AAHX) were generally practical for radon control only in those houses or zones of houses that have low to moderate initial radon levels and ventilation rates. Finally, the success of another mitigation system based on pressurizing the basement depends on achieving a pressure in the basement that is at least 2 to 3 Pa greater than the average wintertime natural depressurization of the basement. Only basements that can easily be maintained air tight therefore are suitable for this system.

Seasonal and annual radon concentrations in all zones and on each level of these houses were measured using mailed alpha-track detectors during the two-year follow-up period. Each house was inspected and the radon mitigation system evaluated during the second heating season of the follow-up study. Some of the systems were modified to eliminate problems which had developed over time.

The alpha-track measurements generally showed an increase in radon levels in a majority of the houses compared to the levels measured immediately after the installation mitigation systems. The greatest increases in radon concentrations occurred in 3 of the 4 houses equipped with basement pressurization systems. In most of the houses equipped with sub surface ventilation systems the radon concentrations also increased over the course of the follow-up period. Radon concentrations in the two houses equipped with air-to-air heat exchangers appeared to depend upon the duration of operation and fan speed settings of the heat exchangers. Factors causing decreased performance of the mitigation system included: (1) a build up of dust and lint on the soil, beneath the slab, at the pipe outlet of subsurface ventilation systems operated in the pressurization mode; (2) noisy and vibrating fans which were turned off by occupants; (3) air-to-air heat exchanger, basement pressurization, and subsurface ventilation system fans which were sometimes turned off or fan speeds reduced by occupants even when there was not a noise problem; and (4) crawl space vents which were closed or sealed.

Monitoring and Evaluation of Radon Mitigation Systems Over a Two-Year Period*

R.J. Prill

In previous research studies, elevated concentrations of radon were found in a significant percentage of the houses located in Eastern Washington and Northern Idaho. A subsequent study, completed in 1986, developed and evaluated radon mitigation techniques and systems in fourteen houses in the area of the Spokane River Valley. This research reports on the performance of these radon mitigation systems for a period of two years.

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Research Division, and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division of the U.S. Department of Energy (DOE) under Contract No. DE-AC03-76SF00098.

Appraisal of the U.S. Data on Indoor Radon Concentrations*

A. V. Nero, K. L. Revzan, and R. G. Sextro

Recent surveys of indoor radon concentrations have suggested that the risk to the U.S. population is much greater than was indicated by earlier surveys. We examine the bases of the discrepancy and show that the interpretations of the recent surveys are in error.

PRE-1984 STUDIES

Results from a number of small surveys were used in 1984 as the basis for developing a U.S. concentration distribution. This analysis discriminated between those surveys undertaken because high indoor concentrations were known or suspected and those that were designed on a

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Division, and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building Energy Research and Development, Building Systems Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

random basis. Furthermore, data taken in the winter were normalized to an approximate annual-average concentration, and the different data sets were weighted by number of houses, region, and population in order to examine the sensitivity of the resulting distribution to these factors. The resulting aggregate distribution, found to be insensitive to weighting, has an average or arithmetic mean (AM) of 55 Bq m^{-3}. Approximately 2% of homes were found to exceed annual-average concentrations of 300 Bq m^{-3}. The distribution was represented well by a lognormal function with a geometric mean (GM) of 33 Bq m^{-3} and a geometric standard deviation (GSD) of 2.8. The annual-average concentration was, on the average, 72% of that measured in the winter. The inclusion of data from areas where concentrations were expected to be higher on the basis of prior information raised the average concentration substantially, as had been expected. A second important survey entailed year-long radon monitoring in 1984-1985 in the homes of 453 physics faculty at 101 universities throughout the United States. The results correspond well to a lognormal distribution with a GM of 38 Bq m^{-3} and a GSD of 2.36. Both surveys utilized data accumulated in living spaces rather than basements, which is a major distinction from the more recent data sets. The fraction of houses with concentrations above 150 Bq m^{-3} are estimated from the earlier survey at 7%, and from the latter survey at 6%. Because of the difference in GSDs, perhaps due to reliance on a particular subpopulation in the latter survey, the functions diverge at higher concentrations; still, the fractions above 300 Bq m^{-3} are only a factor of two apart.

RECENT STUDIES

In one study, Alter and Oswald find that approximately 60,000 U.S. etched-track measurements are found to average 266 Bq m^{-3}. However, 50,000 of the data are from only 6 states, including some known to have high concentrations. Removing the data from these states yields an average, for the 10,251 remaining data, of 158 Bq m^{-3}. Two alternative methods of obtaining a more representative selection yield averages of 152 and 153 Bq m^{-3}. The authors find this convergence striking, assert that the results provide a rough "exposure" estimate, and conclude that the national "exposure" exceeds the 55 Bq m^{-3} cited previously. In fact, even the three restricted sets of data are likely to overrepresent homes with high concentrations. Further, the parameter of interest for indoor exposures is the annual-average concentration in the living space.

A major difficulty is that a large portion of the measurements are performed in basements. Concentrations in basements average approximately twice those on first floors during the winter, with an even larger ratio during the summer. In fact, for a subset of measurements for which location was recorded, the 44% taken in basements have an average concentration 2.0 times the average from the non-basement readings. If we attempt to correct an apparent average of 155 Bq m^{-3} to a living-space average assuming that 44% have results that are a factor of 2 high, we find a corrected average of 108 Bq m^{-3}. It is even more difficult to quantify the effect of oversampling in areas or houses where high concentrations are known or suspected. We note that a 25% reduction of the AM yields 81 Bq m^{-3}; there are indications from the etched-track data themselves and from comparison with the EPA data discussed below that the effect of oversampling is at least this large. Finally, a preponderance of measurements are performed during winter only. As indicated above, annual-average concentrations have been found to average approximately 72% of winter values. Given probable mixes of seasons in which the etched-track measurements were taken, the annual-average concentration may therefore be 80 or 90% of the value above, i.e., approximately 69 Bq m^{-3}. These considerations are enough to indicate that an average less than 75 Bq m^{-3}, reasonably consistent with the earlier surveys, is probable.

Alter and Oswald also find that 23% of the 10,251 data exceed the EPA remedial level of 148 Bq m^{-3}. However, a lognormal function with a GM of 61 Bq m^{-3} and a GSD of 3.2 is found to fit the data below 148 Bq m^{-3} very well, with a considerable excess of data above this point, particularly of very high values. The considerations discussed in the previous paragraph account for this excess.

A second data set has arisen from recent efforts of the EPA in conjunction with 10 states. During the winter of 1986-1987, charcoal detectors were deployed in statistically chosen samples of homes in nine states, plus another state in which volunteers were relied on. Examining the EPA press material, one finds the following information: the number of homes monitored in the main sample varied from 190 to 1787 for the ten states, totaling approximately 10,000. The AM for the main sample was 110 Bq m^{-3}; 20% of measurements exceeded 148 Bq m^{-3} and approximately 1.1% exceeded 740 Bq m^{-3}. Measurements were performed following the EPA screening protocol so that, as indicated in some of the EPA backup material, these results - taken in winter and, often, in basements - do not represent annual-average concentrations to which people are exposed. Nonetheless, the press reports, following the EPA press release, compared these results directly with the EPA action guideline and indicated that 21% of the homes exceeded the guideline, an inappropriate use of the data.

If the correction from basement concentrations described above is made to the AM of 110 Bq m^{-3}, and the resulting 76 Bq m^{-3} is corrected to an annual-average using the factor of 0.72, an AM of 55 Bq m^{-3} is found. The precise agreement with previous results is fortuitous, but indicates that - if proper adjustments could be made - agreement would be quite satisfactory. Furthermore, these adjustments would drastically reduce the fractions above 148 and 740 Bq m^{-3}, apparently to the vicinity of the early results, which were that 6 or 7% of homes exceed 148 Bq m^{-3} and perhaps 0.1% exceed 740 Bq m^{-3}.

Any two probabilities may be used to define a lognormal distribution. The particular distribution which passes through the given probabilities for 148 and 740 Bq m^{-3} has a GM of 58 Bq m^{-3} and a GSD of 3.0, which implies an

AM of 106 Bq m^{-3}, which is close enough to the actual AM to suggest that the lognormal may be a useful representation of the data. If so, then lognormality is maintained at least to the region of 740 Bq m^{-3}, which contrasts with the data of the Alter-Oswald study. Both the GM and the GSD of the distribution are higher than those of the early surveys, of course, but we have shown that they have been overestimated. Extrapolation of the lognormal indicates that 0.01% of the homes, i.e., 1 home, should exceed 3700 Bq m^{-3}. The actual number is 3, so that we expect that fewer than 3 in 10,000 homes exceed this level, which is a much smaller fraction than has been suggested.

CONCLUSIONS

Monitoring efforts undertaken before 1985 indicate that the radon concentration in U.S. houses averages approximately 55 Bq m^{-3} and that, in approximately 6%, annual-average levels exceed 150 Bq m^{-3}, with perhaps 1-2% having 300 Bq m^{-3} or more. However, several recent large-scale data sets yield average concentrations of 100-150 Bq m^{-3}, with perhaps 20% of results exceeding 150 Bq m^{-3}, leading to an exaggerated estimate of risk. In fact, these recent data sets overrepresent high-concentration houses or include sampling performed in basements or in the winter only. Adequate information is not available to adjust these results precisely to annual-average indoor concentrations experienced by the population, but plausible corrections yield results that are consistent with the distributions previously found.

Parametric Modelling of Temporal Variations in Radon Concentrations in Homes*

K.L. Revzan, B.H. Turk, J. Harrison, A.V. Nero, R.G. Sextro

The radon concentrations in the living area, the basement, and underlying soil of a New Jersey home have been measured at half-hour intervals over the course of a year, as have indoor and outdoor temperatures, wind speed and direction, and indoor-outdoor and basement-subslab pressures; in addition, periods of furnace operation have been logged. We generalize and extend an existing radon entry model in order to demonstrate the dependence of the radon concentrations on the environmental variables and the extent of furnace use. The model contains parameters which are dependent on geological and structural factors which have not been measured or otherwise determined; statistical methods are used to find the best values of the parameters. The non-linear regression of the model predictions (over time) on the measured living area radon concentrations yields an R^2 of 0.88.

Theory

We assume that a house is divided into two zones, the basement and living area, of which only the former is in contact with the soil; the house is assumed to be depressurized as a result of temperature differences between inside and outside and the flow of wind around the structure. On the basis of a highly simplified model, we represent the soil gas radon concentration, C_s, as

$$C_s = p_1 (1 - \exp[-p_2/\Delta p_s]), \tag{1}$$

where the p_n are parameters which depend on the properties of the soil and on the nature of the openings between basement and soil and Δp_s is the pressure across the soil.

From the mass-balance, assuming the outdoor radon concentration to be negligible, the steady-state radon concentration in the basement is

$$C_b = (f_{sb}C_s + f_{lb}C_l) / (f_{bo} + f_{bl}), \tag{2}$$

where C_b, C_l, and C_s are the radon concentrations in the basement, living area, and soil, respectively, and f_{sb}, f_{lb}, f_{bo}, and f_{bl} are the flows from soil to basement, living area to basement, basement to outside, and basement to living area, respectively, and where the outside concentration and diffusive entry have been neglected. Similarly, the steady-state living area concentration is

$$C_l = f_{bl} C_b / (f_{lo} + f_{lb}), \tag{3}$$

where f_{lo} is the living area to outside flow.

We now assume that the flow from living area to basement, f_{lb}, is entirely due to furnace operation, that the flow from basement to living area is the sum of f_{lb} and a term directly proportional to the flow from the living area to the outside, and that the basement to outside flow is a constant multiple of the living area to outside flow, so that

$$C_b = \frac{f_{sb} C_s (1 + p_3A_f)}{(p_4 + p_5A_f)f_{lo}}, \tag{4}$$

and

$$C_l = (p_6 + p_7A_f) C_b / (1 + p_7A_f) \tag{5}$$

where A_f is the fraction of the time the furnace is in operation. When the furnace is not in operation, C_b is the quotient of a source term and the outside to basement flow; when the furnace is in operation, assuming the fur-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division and by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Research Division of the U.S. Department of Energy (DOE) under Contract No. DE-AC03-76SF00098. It was also supported by the Office of Environmental Engineering Technology Demonstration, Office of Research and Development of the U.S. Environmental Protection Administration (EPA) through interagency agreement DW89931876-01-0 with DOE.

nace flow to dominate other flows between the two interior zones, the denominator becomes the total flow into the house. With the furnace off, the house can be represented by the two-zone model; with the furnace on, the air of the two zones is mixed and the house is effectively a single zone.

If we now represent the flows appearing in equations 4 and 5 by

$$f_{sb} = p_8 \Delta T + p_9 u^2; \quad f_{lo} = (p_{10} \Delta T + p_{11} u^2)^{0.5}, \qquad (6)$$

where ΔT is an appropriate temperature difference and u is the wind speed, and if we further assume that Δp_s is proportional to f_{sb}, then we have a model in which the only independent variables are the temperature difference, the wind speed, and the fractional furnace operation. There are 3 parameters in the equations determining C_s (1 and 6), 6 in those determining C_b (1, 4, and 6, with terms collected), and 2 in that determining C_l (5).

Results

We shall apply the model to a two-story dwelling with a basement located in north central New Jersey, which was selected as the control for a year-long study of the effectiveness of remedial action in six other houses in the same general area. The basement is almost entirely below grade; it contains a forced-air furnace whose ductwork has been observed to be leaky. Radon concentrations were measured in the soil below the basement slab, in the basement itself, and on the first floor using continuous radon monitors. Environmental measurements included indoor, outdoor, and soil temperatures, wind speed and direction, barometric pressure, and precipitation. Differential pressures were measured between the top and bottom of the basement slab, between the first floor and the basement, and across the four walls separating the basement from the outside air. Furnace operation was measured on a binary (on/off) basis. Data was collected for 10 months, beginning on 18 September 1986; all data was logged automatically at half-hour intervals. The comparison between theory and experiment is, however, based on three-day averages of the data.

A linear regression shows that Δp_s is directly dependent on ΔT, u, and possibly on A_f, but it is impossible to determine statistically which of the variables must be included in the equation. The best results occur when we use the basement temperature, the soil temperature at 70 cm depth, and the furnace activity; the R^2 is 0.82. If the same variables are used to predict C_s, we find an R^2 of 0.62. The model accounts for the general tendency of the data, but is insufficient to account for the day-to-day fluctuations. There may be inhomogeneities in the soil gas concentration in the vicinity of a house, in which case a spot measurement could be unrepresentative of the average and the model would not be expected to predict well.

The basement concentration data can be divided into three distinct periods: two periods of warm weather during which relatively large fluctuations in concentration occurred and the winter period, running from December 4 through March 12, during which the fluctuations were relatively small. The difference in character between the warm and cold weather periods may be due to freezing of the soil. When we model the basement concentration using equations 4, 6, and 7 with C_s equal to its measured value, the fit is quite poor, suggesting that the soil gas measurement is not representative. When we use equation 1 to represent the soil gas, the fit to the data for the full year is poor, but some success is found in fitting distinct equations to the data for the warm and cold weather periods taken separately. The best fit to the warm weather data is obtained when the basement-outside temperature difference and the wind speed are used in both the source and removal terms; the R^2 is 0.63. The best fit to the cold weather data is obtained when the basement-soil temperature difference and the furnace activity are used in the source term; the R^2 is 0.70. The comparison of theory and data for the basement reveals the inadequacy of the theory; one major flaw may be the inability of the theory to represent the flow across the building shell (the air exchange) correctly.

When the measured values of C_b are used in equation 5, we find p_1 and p_2 to be 0.24 and 5.1, respectively, with an R^2 of 0.93; we regard this result as confirming the theory leading to that equation. When the calculated values of C_b are used, we find an R^2 of 0.88, which is satisfactory, but we note that the prediction of the basement concentrations is not good, and the result may be fortuitous.

Technique for Measuring the Indoor ^{222}Rn Source Potential of Soil *

W.W. Nazaroff and R.G. Sextro

Elevated indoor radon concentrations are often caused by high rates of entry of radon generated in soil within a few meters of a building's substructure. The potential of soil for generating high indoor radon concentrations depends on two factors: (1) the rate of release of radon from soil grains into the pore space of the soil, and (2) the volume of soil that can contribute its emanated radon to indoor air. The aim of this work is to develop techniques for measuring these factors and a method for combining

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Research Division, and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division of the U.S. Department of Energy (DOE) under Contract No. DE-AC03-76SF00098. It was also supported by the Office of Radiation Programs, of the U.S. Environmental Protection Agency (EPA) through Interagency Agreement DW89932609-01-0 with DOE.

the results into a single indicator of the indoor radon source potential of soil.

The experimental method entails installing a sampling probe into the soil. A pump is used to extract air from the soil through the probe, and a sample of this air is analyzed to determine its radon content. From this measurement, the rate of release of radon into the soil pores can be determined. The difference in air pressure established by the pump is measured between the tip of the probe and the atmosphere, and the rate of air flow through the probe is also measured. From these parameters, and the dimensions of the probe, the permeability of the soil is computed. This characteristic indicates how much soil may contribute radon to the interior of a building.

A theoretical analysis of radon transport in soil is developed as a basis for interpreting the experimental data and for combining the results into a single indicator of radon source potential. In the analysis, it is first argued that, for homogeneous soil, molecular diffusion may be neglected compared with bulk flow as a radon transport mechanism in cases in which the source potential is high. Then, equations for the pressure field and the radon flux are formulated and solved numerically for two idealized soil cavities with reduced air pressure (1) an isolated sphere, and (2) a long cylinder with a horizontal axis. The first case represents the soil sampling probe, and the latter case is a model for a house in which there is a leakage path from the soil around the basement perimeter, such as a floor-wall gap or crack.

In a preliminary field test, the measured indoor radon source potential in soils adjacent to four New Jersey houses was found to correlate well with the measured average indoor radon concentrations.

Successful preliminary tests suggest that this may be a useful basis for setting priorities in efforts to identify individual houses with high concentrations. The method could also be used to determine whether construction practices in an area need to be modified to prevent elevated radon concentrations in future housing. Further survey work must be conducted comparing measured indoor radon concentrations with the indoor radon source potential of nearby soil. Ultimately, the demonstration of a strong empirical correlation between the higher observed indoor concentrations and the source potential is both sufficient and necessary to justify the use of this method for appraising the risk of high indoor radon concentrations from soil.

Mapping Surficial Radium Content as a Partial Indicator of Radon Concentrations in U.S. Houses

K.L. Revzan, A.V. Nero, R.G. Sextro

In connection with the problem of indoor radon, we discuss the use of data from the National Aerial Radiometric Reconnaissance to develop maps of radium in soil, at various resolutions, for the contiguous 48 states. We examine the relationship between the results of measurements of radon in houses and the indications of the U.S. map, noting that some, but by no means all, of the areas known to have elevated radon concentrations appear as areas of higher radium concentration than their surroundings and that there are other areas, in which measurements of high radon levels have not been made, which are suggested as deserving of interest. We discuss mapping techniques for smaller areas and possible methods of dealing with apparent discrepancies between adjacent areas.

Results of Mapping

An important factor determining radon concentrations in houses is the radon concentration in the pore spaces of the underlying soil. For that reason, a useful first step in the identification of areas of elevated radon is the development of a map of soil gas concentration or, what is equivalent, a map of radium concentration in soil, for the U.S. Though such a map cannot *exclude* any area of the country from the possibility of having houses with high radon levels (since, for example, high permeability soil may allow transport of sufficient soil gas of low radon concentration to produce a high indoor concentration), it can suggest certain areas which are likely to have large numbers of those houses.

The necessary data for a radium map was obtained by the National Aerial Radiometric Reconnaissance (NARR), which measured the gamma radiation from the top 0.5 m of soil or rock in order to discover uranium deposits. From the data of this survey, obtained and processed by a number of subcontractors, a database of manageable size was developed, in which we have stored the average radium concentration for each 1.6 km along the survey flightlines. A map of the contiguous 48 states was then

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Division, and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division of the U.S. Department of Energy (DOE) under Contract No. DE-AC03-76SF00098. It was also supported by the Office of Radiation Programs of the U.S. Environmental Protection Agency (EPA) through Interagency Agreement DW89932609-01-0 with DOE. This report has not been subjected to EPA review. Its contents do not necessarily reflect the views of EPA, nor does mention of firms, trade names, or commercial products constitute endorsement or recommendation for use.

created, on which a dot has been placed in each 20 × 20 km area, the size of the dot representing the average radium concentration in that area.

The map reveals that certain areas appear sufficiently different in character from their surroundings to lead to suspicion that there might be problems involved in attempting to compare data obtained by different subcontractors despite their use of the same calibration procedures. The problem is perhaps most clearly exhibited in the Rawlins and Greeley quadrangles of Wyoming and Colorado. The means of Ra for the two quadrangles are 6.3 and 8.1 Bq kg^{-1}, while the mean Ra of the six surrounding quadrangles is 33.3 Bq kg^{-1}. Other possible calibration anomalies appear in southwestern South Dakota, eastern Washington and western Idaho, and San Jose, California. The average radium concentration of the territories surveyed by individual subcontractors ranges from 20 to 32 Bq kg^{-1}, but the variation may be explained, at least in part, by the different areas of the country flown by each; the question of the importance of subcontractor performance remains open.

The following areas, which the map reveals as having high radium concentrations compared to their surroundings, have also been found to have high radon concentrations in homes: eastern Pennsylvania-northern New Jersey (Reading Prong), eastern Tennessee-western North Carolina, western Washington-eastern Idaho (Spokane-Cour d'Alene), and western Florida (phosphate-bearing land). Apart from Florida, where the situation is well understood, and Tennessee, the mean levels of radium in these areas, while higher than their surroundings, are not high in absolute terms, and the nature of the relationship between the means of radium in soil and radon in houses remains to be established.

One region is known to have high radon concentrations but does not appear to have high radium levels: the Red River valley of North Dakota. While the map shows the valley to be somewhat higher in radium than the territory to the east and west, the level is the same as that of the territory to the south, so that it is difficult to infer that this might be a region of interest. There are a number of areas which, conversely, have high radium concentrations but in which high radon levels have not been found: central California, southern Arizona-New Mexico, a number of regions in the Rocky Mountain states, central New Hampshire-southern Maine, and, most conspicuously, southwestern South Dakota. Some of these are known to be areas in which uranium deposits occur; some, as we have suggested, may stand out because of calibration problems; some may be worthy of investigation.

The Statistics of Radium in Soil

On the basis of the 22,172 average radium concentrations used for the U.S. map, the geometric mean (GM) is 25 Bq kg^{-1}, the geometric standard deviation (GSD) is 1.6, the arithmetic mean (AM) is 27 Bq kg^{-1}, and the arithmetic standard deviation (ASD) is 12 Bq kg^{-1}. These parameters are useful for making comparisons among regions, but they are misleading in that each datum is treated as if it were itself an observation rather than as an average of original observations. Since we have retained the number of observations, the AM, and the ASD for each 1.6 km flightline datum, it is a simple matter to calculate an ASD for each 20 × 20 km region and then, to calculate an ASD for the contiguous U.S. On the basis of the original 24,591,855 measurements, this ASD is 21 Bq kg^{-1}. Calculation of the GM and GSD on the same basis involves approximations, since we have not retained the GM and GSD of the observations in our database. If we assume the data to be lognormally distributed, however, we may use the AM and ASD to calculate a GM and GSD: 21 Bq kg^{-1} and 2.0, respectively.

If we now consider that each original observation itself represents an integration of several hundred square feet and that large areas of the country remain unobserved due to the relatively large distances between flightlines, it is apparent that the actual GM of observations of radium in soil made at ground level, each representing an area the size of a house, is likely to be somewhat greater than 2.0. The GM of measurements of radon concentration in houses in the U.S. is approximately 2.8. Suppose that the indoor radon concentration is the product of the soil gas radon concentration, represented by the radium concentration, and some other lognormally distributed factor or combination of factors. Given the fact that the logarithms of GSDs add in quadrature, two factors contributing equally to the variation in radon would each have a GSD of 2.1, which is very close to the calculated GSD for radium. On this basis, the observed variation in radium in soil accounts for roughly half the observed variation in indoor radon.

It is clear, however, that we must look to factors other than radium in soil to explain the radon concentration data. In part of Eastern Pennsylvania, for example, we find a GM indoor radon concentration of 120 Bq m^{-3} (with a GSD of 3.4), which is a factor of 3.6 higher than the national GM. The GM radium for this area is generally 20-40 Bq kg^{-1}, with a high of 56 Bq kg^{-1}; the GSD is generally 1.5-2.5. If the relationship between radium and the other factors affecting radon in houses were to be the same in Eastern Pennsylvania as in the contiguous 48 states as a whole, the GM radium should be on the order of 75 Bq kg^{-1} and the GSD should be 2.4.

Conclusions

We have shown that, on a national basis, as much as half the variation in radon from region to region may be accounted for by the level of radium in the soil, but that there are regions for which the radium concentration does not account for the relatively high observed radon.

Indoor Atmospheric Chemistry: Interactions of Radon with other Gaseous Pollutants *

J.M. Daisey, R. Sextro, A.T. Hodgson, N. Brown, and D. Lucas

Research was initiated on the radiolytic interactions of radon and radon progeny with other gaseous indoor pollutants. The objectives are to chemically characterize the gaseous and particulate products generated by the radioactive decay of radon and its progeny, to determine formation rates and size distributions of the aerosols and resultant equilibrium factors and to elucidate reaction mechanisms.

Three environmental chamber experiments were conducted for the purpose of determining appropriate experimental parameters. These experiments were conducted in collaboration with P.K. Hopke and M. Ramamurthi, University of Illinois.

The chamber was spiked with a mixture of volatile organic compounds (VOC) and radon. VOC and radon decay rates, over and above chamber background (determined in a separate chamber experiment), were monitored for 42 hours. The activity size distribution of the ultrafine aerosol was measured with a multi-screen sampler. Four VOC were used: n-hexane, toluene, 2,3-dimethyl-2-butene, and limonene. The 2,3-dimethyl-2-butene had a *net* decay rate of 0.007 h^{-1}. The limonene decayed at a net rate of 0.004 h^{-1}. The decay rates for the other two compounds were not significantly different from those measured in the absence of radon. In this experiment, there was no evidence of formation of ultrafine aerosol; however, it was determined that n-butanol from the condensation nucleus counter had back diffused into the chamber. This compound is a free radical inhibitor and contamination of the chamber with the n-butanol probably accounts for the lack of particle formation in contrast to the first experiment.

A molecular beam mass spectrometer is being modified and evaluated to allow for the detection and quantification of ions produced by the radioactive decay of radon and its progeny in indoor air. The apparatus had previously been used to measure neutral species in transient combustion events, using electron-impact ionization and analog signal detection and averaging methods. Many significant changes are needed in the beam system to permit the detection of the low concentrations of ions that are expected in these experiments.

*This research is supported by the Director, Office of Energy Research, Office of Health and Environmental Research, under Contract No. DE-AC03-76SF00098.

Initial Efficiencies of Air Cleaners for the Removal of Nitrogen Dioxide and Volatile Organic Compounds *

J.M. Daisey and A.T. Hodgson

The objective of this research was to investigate the effective cleaning rates (ECRs) of selected portable air cleaners for removing NO_2 and volatile organic compounds from air when first exposed to concentrations typical of those found indoors. The ECR represents the air volume per unit time from which a contaminant has been removed and is useful in evaluating the cleaning effect in rooms of different sizes. We used NO_2 and VOC because they have documented adverse health effects and are commonly found at elevated concentrations in residences.

Four portable air cleaners were selected for study. All incorporated some activated carbon. Two devices designated PF1 and PF2 had multiple stage filter cartridges employing glass fiber mats for particle removal. The PF1 air cleaner had a layer of finely divided carbon impregnated in a fibrous mat and had the least amount of carbon. The PF2 unit had a layer containing activated carbon pellets (115 g) and a catalyst (99 g). The ES unit had a HEPA filter for particle removal, and contained the largest amount of activated carbon (~130 g) which was combined with potassium permanganate (~90 g). The fourth device, EP, removed particles by electrostatic precipitation rather than filtration and had 55 g of activated carbon.

Experiments were conducted in a 20-m^3 environmental chamber operated without mechanical ventilation. The chamber was ventilated and then the NO_2 and VOC were added to the chamber and mixed. The air cleaner was turned on and the rate of decay of the compounds was determined. Removal efficiencies for NO_2 were determined at an initial chamber concentration of ~500 $\mu g\ m^{-3}$. Six VOC, representative of five major classes of VOC typically found in indoor environments were used: n-heptane, an aliphatic hydrocarbon; toluene, an aromatic hydrocarbon; dichloromethane (methylene chloride) and tetrachloroethylene chlorinated hydrocarbons; hexanal an aldehyde; and 2-butanone (methylethylketone) a ketone. The average initial chamber concentrations for these compounds ranged from 130 to 680 $\mu g\ m^{-3}$.

None of the air cleaners removed dichloro- methane. The initial ECRs for NO_2 and the remaining five VOC (averaged for the VOC) for the four air cleaners are shown (figure). The ES and PF2 devices were reasonably effec-

*This work was supported by the U.S. Consumer Product Safety Commission under Contract No. CPSC-IAG-86-1259 and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Buildings Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

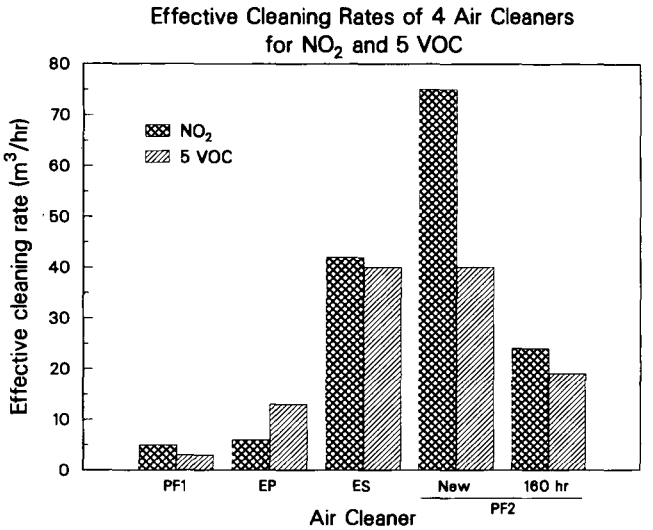


Figure Initial effective cleaning rates of four air cleaners for NO_2 and five VOC (average). Effective cleaning rate for the PF2 air cleaner after 150 hours of operation in a house is also shown.

tive initially in removing NO_2 and the five VOC. Removal rates were equal to one air change per hour or more for a room of about 40 m^3. The PF2 device, which had a catalyst as well as carbon, had the highest ECR for NO_2 and was almost twice as effective in removing NO_2 as was the ES unit. These two devices had relatively high air flow rates and the most carbon. The PF1 and the EP devices, had much lower ECRs for the removal of NO_2 and VOC and would not effectively remove these pollutants from even a small room.

The PF2 air cleaner was subsequently operated, with the same filter, for 2.5 months (150 hours) in an older residence of non-smokers who used a gas range for cooking. The air cleaner was then tested a third time in the chamber. The figure compares the ECRs in the first and third experiments. For NO_2, the ECR was reduced to about one-third of the initial value. For the five VOC removed by the air cleaner, the ECRs after field operation were about half the initially measured values. The product literature for this device states the estimated filter life is about 1000 hours.

Further investigation is needed to determine ECRs and efficiencies over periods of extended use for air cleaners which have relatively high ECRs. Investigation of possible chemical reactions occurring with extended use is also warranted.

Volatile Organic Compounds in Large Buildings *

J.M. Daisey and A.T. Hodgson

There have been increasing numbers of complaints about discomfort and illness in new and newly renovated office buildings. This increase in complaints has been correlated with reduction in ventilation for energy efficiency and increased uses of synthetic building materials and furnishings. Exposures to volatile organic compounds (VOC), originating from materials and furnishings and various products used in large buildings are suspected to play a role. However, there has been relatively little research to characterize VOC in large buildings, to identify their sources, to evaluate temporal and spatial variations in VOC concentrations or the effects of building ventilation on concentrations.

The purposes of the ongoing study of VOC in large buildings are: 1) to develop a data base of concurrent measurements of VOC concentrations and ventilation; 2) to investigate both short- and long-term temporal variations in source strengths of VOC; and 3) to develop methods to identify major sources and estimate their contributions to indoor VOC concentrations.

To date, simultaneous measurements of VOC and of ventilation have been made in four large office buildings, a museum-teaching facility and a school. Concentrations of total organic carbon in these buildings have ranged from less than 1 to 11 $mg\text{-}m^{-3}$.

Temporal variations in indoor concentrations of VOC and the effects of ventilation on VOC have been under detailed investigation in a large seven-story office building in Portland, OR in collaboration with R. Grot, National Institute of Standards and Technology. The first measurements were made in August, 1987, before the building was completely finished but after it was partially occupied. Subsequent VOC samples have been collected on three occasions over a period of a year. In addition, samples of major materials used to finish the interior have been collected and screened for VOC emissions.

The concentrations of VOC and total organic carbon in the Portland building have varied considerably over the study, with the highest concentrations observed when the ventilation rate was lowest. The concentration and ventilation rate data were used in a single-equation mass balance model to estimate specific source strengths and to determine if these had declined as expected over time. The results showed that the source strengths of the individual VOC and of total organic carbon remained relatively

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Buildings Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098 and by the National Bureau of Standards under Interagency Agreement No. BG-130(01).

constant over the course of the study. The dominant source of the VOC in this particular building appears to be, not the interior finish materials, but a solvent-using activity in the building. Efforts to estimate the contribution of this activity to indoor concentrations are in progress. The emission of total organic carbon in this building was estimated to be over 2.5 kg per 8-hour day.

Development of a Sampling and Analysis Method for Polycyclic Aromatic Compounds in Indoor Air *

J.M. Daisey, L.A. Gundel, A.T. Hodgson, and F.J. Offermann†

Research was initiated to develop a method for sampling and analyzing vapor- and particulate-phase polycyclic aromatic hydrocarbons (PAH) and nitro-PAH in indoor air. Many of the PAH and nitro-PAH are carcinogens in animals but there have been few indoor measurements of these compounds. Efforts to measure these compounds in indoor air have been hampered by the lack of sensitive, validated sampling and analytical methods. For indoor air, the sampling rate must be much less than the air exchange rate so that the act of sampling has a minimal impact on the concentrations of indoor pollutants which are removed by the sampling.

The approach being taken in this research is to develop and validate a sampler consisting of a filter followed by an XAD-4 resin bed to collect, respectively, particulate and vapor phase PAH and nitro-PAH. Approximately 25 m^3 of air will be sampled in 12 hours. After solvent extraction, the vapor phase compounds will be analyzed by gas chromatography-mass spectrometry and the particulate phase compounds will be analyzed by high pressure liquid chromatography with fluorescence detection. The methods will be field tested in selected houses.

*This work was supported by a contract from Indoor Environmental Engineering and the California Air Resources Board.
†Indoor Environmental Engineering, 3400 Sacramento Street, San Francisco, CA 94118

The Role of Heterogeneous Reactions of NO_2 in Indoor Air *

J.M. Daisey and L.A. Gundel

Concentrations of NO_2 in indoor air can be one to two orders of magnitude greater than those in outdoor air if combustion sources such as gas stoves are present. Indoor surfaces have been shown to remove NO_2, and in a few instances, to convert it to NO. The purpose of this study was to determine if heterogeneous reactions of NO_2 on surfaces of materials in indoor environments could produce other secondary pollutants which might be hazardous or which might initiate further indoor atmospheric chemistry.

Experiments were conducted in a specially designed and constructed annular reaction vessel containing selected indoor materials: wool or nylon carpet, polyurethane foam or wallboard paper. NO_2, at concentrations of 1 ppm or less, was passed through the vessel in dry or humid (50% relative humidity) air. Concentrations of NO_2, NO, HONO, and HNO_3 were measured downstream of the reactor. An annular denuder was used to collect the acidic gases, HONO, HNO_3.

Each material removed a large fraction of the incident NO_2. The polyurethane foam removed all of the NO_2 in the air stream during the initial exposure period, but after about 5 hours was saturated. Nylon and wool carpet removed about 35% and 50%, respectively, of the incoming NO_2. NO was produced in varying amounts on all of the four materials investigated.

Significant quantities of gas phase nitrous acid (HONO) were produced from the interaction of NO_2 with both the foam and the wool carpet. Much smaller quantities of nitric acid (HNO_3) were produced. The excess of HONO over HNO_3 indicates that a direct reaction with these materials, rather than a disproportionation in sorbed surface water, has occurred. On foam, in humid air, at least 7% of the initial NO_2 (560 ppb) was converted to HONO, at a rate of about 0.5% per hour. For wool carpet, the conversion rate was only about 0.1% per hour.

The results of the experiments on heterogeneous reactions on surfaces of indoor materials have demonstrated that nitrous acid can be generated in indoor environments at substantial rates. The presence of this secondary pollutant may lead to subsequent indoor atmospheric chemistry and/or may pose some health hazard in itself.

*This research is supported by Exploratory Research and Development Funds from the Lawrence Berkeley Laboratory.

Transport of Volatile Organic Compounds from Soil into a Residential Basement*

A.T. Hodgson, K. Garbesi, R.G. Sextro, and J.M. Daisey

For residents of nearby houses, landfills are potentially important sources of exposure to toxic volatile organic compounds (VOC). Even municipal landfills accepting only nonhazardous material have been found to contain air concentrations of VOC high enough to cause concern. If not properly contained, VOC can migrate through the soil by aqueous or gas-phase transport. Gaseous compounds in the soil around houses are available for transport into these houses.[1]

Our investigation sought to identify the mechanisms involved in transport of VOC from soil gas into the basement of a house situated in an area of contaminanted soil. The study site was a single-family house adjacent to a covered municipal landfill in California. We had found previous evidence of migration of gas and VOC to the site from a landfill 70 m from the house at its closest point. The house was built over a basement which was almost entirely below grade. The foundation and basement consisted of a cement-block wall built on a cement slab. Experiments were conducted at the site over a four month period during the dry season.

Thirty soil probes were installed around the house at distances ranging between 0.5 to 12 m from the basement wall. The majority of these probes terminated at a depth of 1.5 m. The in situ permeability of the soil measured at the soil probes averaged 2×10^{-10} m^2.

Samples of soil gas, outdoor air, and indoor air for qualitative and quantitative analyses of VOC were collected on multisorbent samplers and analyzed by gas chromatography-mass spectrometry. The VOC identified in soil gas were predominantly halogenated and oxygenated compounds, a number of which have been detected in landfills. The dominant compounds in soil gas were Freon-11, Freon-12, tetrachlorethylene, dichloromethane, and acetone. Many of the compounds in soil gas were also measured in indoor air but at much lower concentrations. Since the house was unfurnished and unoccupied and had no other obvious sources, soil gas was assumed to be the primary source of most of these compounds.

The entry rate of soil gas into the basement was estimated as a function of basement depressurization. Pure SF_6 was injected into the soil around the house to provide a source of labeled soil gas. One month later, after the SF_6 had diffused over most of the site, the soil-gas concentrations of SF_6 and Freon-12, a soil-gas contaminant, were measured at the soil probes nearest the basement. Then, with the basement closed, the exhaust fan was operated to produce pressures in the basement of -20, -30, -40, and -50 Pa relative to ambient pressure. Concentrations of SF_6 and Freon-12 in basement air were continuously monitored throughout the experiment. The entry rate of soil gas at each depressurization stage was estimated from the concentration data using a simple mass-balance model, assuming steady-state conditions. The slopes of the regression lines of entry rate versus basement depressurization diverged for SF_6 and Freon-12 undoubtably due to differences in their distributions around the house and the consequent uncertainties in the average soil gas concentrations of the two compounds. However, the regressions suggest that for this house the entry rate of soil gas due to pressure-driven flow would be less than 1 m^3/h at a typical basement depressurization of a few Pascals resulting from wind and an indoor-outdoor temperature differential. For comparison, the infiltration rate of outdoor air for the house at typical winter conditions would be about 500 m^3/h.

Since the basement of this house was well coupled with the soil and the soil was moderately permeable, the pressure-driven entry of soil gas was probably limited by the low below-grade leakage area of the basement. However, for houses with greater below-grade leakage areas, soils of equal or greater permeability, and low infiltration rates, the relative contribution of pressure-driven inflow to the total inflow of air can be much higher. Therefore, it is concluded that advective transport can result in elevated indoor concentrations of soil-gas VOC in those houses which have high relative inflow rates of contaminated soil gas.

REFERENCE

1. Nazaroff WW, Lewis SR, Doyle SM, Moed BA, Nero AV Nero. Experiments on pollutant transport from soil into residential basements by pressure-driven airflow. *Environ Sci Technol* 1987; 21: 459-466.

*This work was supported by the Occidental Chemical Corporation under agreement BG8602A and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The Indoor Environment of Commercial Buildings*

D.T. Grimsrud, J.T. Brown, W.J. Fisk, J.R. Girman

The primary focus of research in indoor air quality has been on residential buildings. This report, by contrast, concentrates on commercial (office and institutional) buildings and is intended for a broad audience ranging from

* This work was supported by the Electric Power Research Institute, Inc. (EPRI) and the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

those who have no previous background in indoor air quality to those with considerable indoor air quality experience.

A recurring theme throughout the report is the sick building syndrome. This troublesome phenomenon, an attribution of the source of general feelings of irritation and malaise to the occupant's building, can cause significant economic damage to the building owners and tenants if the productivity of the workforce declines. Considerable uncertainty exists regarding the cause or causes of sick building syndrome. Current research on indoor air quality issues in commercial buildings concentrates on sick buildings; however, one must be careful not to overemphasize this topic. The health outcomes associated with the sick building syndrome tend to be short-term irritation effects. Longer-term, chronic effects associated with exposure to pollutants in commercial buildings may be equally or more important. These are not addressed typically in any study focused on the sick building syndrome. Where long-term effects are understood, they are discussed in this report.

The report is divided into seven chapters. The introductory chapter is followed by a discussion of the effects of initial design decisions that affect air quality. Many of these design decisions pertain to the ventilation systems. The mechanical ventilation systems, rare in residences but common in commercial buildings, have been identified by some as major causes of problems in the indoor environment. Their influence on indoor air quality is treated in chapter three.

Pollutants present in commercial buildings are discussed in chapter four. The discussion is organized by pollutant classes arranged in order of the expected pervasiveness of the pollutant problem. The long pollutant chapter is followed by the three final shorter chapters examining human factors, investigative procedures, and general corrective procedures to be considered when problems are discovered.

Pacific Northwest Existing Home Indoor Air Quality Survey and Weatherization Sensitivity Study*

B.H. Turk, D.T. Grimsrud, J.Harrison, R.J. Prill, and K.L. Revzan

The study reported in this paper had the following objectives:

1) survey indoor pollutant concentrations in unweatherized Pacific Northwest housing,

2) study the effect of weatherization on indoor pollutant levels.

SCREENING SURVEY

A screening survey of indoor air quality in 111 unweatherized houses was followed by staged weatherization in 40 of these 111 structures. Study sites were located in two of the three major climate areas of the Bonneville Power Administration (BPA) region. Houses in Portland and Vancouver, WA are found in the mild, coastal region while houses in Spokane and Coeur d'Alene, Idaho are located in located in the high plateau desert region east of the Cascade Mountains. Passive samplers to measure concentrations nitrogen dioxide, water vapor, formaldehyde, and radon were mailed to homeowners who put them in place using the shipping box as the sampler holder. Extensive telephoning was required to assure that instructions were followed. The screening survey results indicate that indoor concentrations of nitrogen dioxide (geometric mean of 5 ppb), formaldehyde (geometric mean of 37 ppb), and water vapor (arithmetic mean of 6.7 g/Kg) were significantly below levels of concern. However, the survey led to the discovery of elevated indoor radon levels in houses in the Spokane River Valley/Rathdrum Prairie of Washington and northern Idaho. The geometric mean concentration for 43 houses in that area was 4.4 pCi/L, compared with other regional and national studies that range from geometric means of 0.8 to 1.0 pCi/L. The high indoor radon levels found in the Valley/Prairie are due to the convective flow of radon-bearing soil gas from a highly permeable soil into the houses.

WEATHERIZATION STUDY

Forty-eight houses from the screening survey were chosen for the weatherization sensitivity phase of the study. Eight of the houses remained unweatherized during the study and acted as control structures; monthly measurements of pollutant concentrations were made in these houses to track the impact of non-weatherization factors on pollutant concentrations. The remaining houses underwent a variety of staged weatherization retrofits: all 40 houses received the standard BPA weatherization package, 14 houses also received wall insulation, while five of the forty houses also received house doctoring. Building and pollutant measurements were obtained using passive samplers where possible, and real-time instrumentation where necessary. Spokane/Coeur d'Alene houses were more tightly sealed against air leakage, both before (geometric mean specific leakage area of 4.9 cm^2/m^2) and after weatherization (geometric mean of 4.1 cm^2/m^2) than the Vancouver area houses (geometric mean of 5.3 and 4.9 cm^2/m^2, respectively). BPA's standard weatherization program reduced the specific leakage area of the 40 weatherized structures approximately 12.5%. The reduction due to wall insulation (6%) was not statistically significant. House doctoring resulted in an additional reduction in leakage area of 26%.

*This work was supported by the Bonneville Power Administration (BPA) under contract no. DE-A179-83BP12921, by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Systems Division of the U.S. Department of Energy under contract No. DE-AC03-76SF00098.

Ventilation rates measured using passive sampling techniques and perfluorocarbon tracers (PFT) had a geometric mean of 0.37 h^{-1} before weatherization, 0.39 h^{-1} after weatherization, and 0.30 h^{-1} after house doctoring; however, these ventilation rates have not been corrected to account for different environmental conditions during the various measurement periods. The PFT-measured ventilation rates averaged approximately 20% lower than ventilation rates calculated using the measured leakage areas, weather data and a predictive model developed at LBL. The PFT technique yields results for a specific set of environmental conditions. The leakage area measurement combined with predictions accounts for environmental conditions but has significant uncertainties due to the reliance of an imperfect model. Because, ventilation rates scale with leakage area, we use the change in the leakage area of the house as the best measure of the change in the ventilation produced by weatherization.

Changes in pollutant concentrations were not well correlated with changes in ventilation rates. Factors other than ventilation, including pollutant source strengths, occupant effects, and environmental conditions are more important in influencing indoor pollutant levels.

While not correlated with changes in ventilation, pollutant concentrations did change. Measured data from this study showed increases of 11% in water vapor concentrations, 1% in formaldehyde concentrations, and reductions of 6% in NO2 and 43% in radon concentrations when the means of the pre- and post-weatherization samples are compared. However, these results represent measurements made during different environmental conditions. Therefore, the results must be corrected to standard conditions if meaningful comparisons are to be made. Simplified models were developed to evaluate the impact of environmental conditions on indoor air pollutants. The models were used to recalculate radon, water vapor, and formaldehyde concentrations from before and after weatherization to corrected standard conditions. The concentrations adjusted to standard conditions show an increase of 8% in post-weatherization water vapor concentration relative to pre-weatherization conditions; a decrease of 3% in formaldehyde concentrations, and a decrease of 33% in radon concentrations. Only the changes in the radon concentrations are statistically significant. Where the radon data are separated by substructure type we find that only in crawlspace houses, where ventilation is added to crawlspaces during weatherization, were the indoor radon levels significantly reduced. Radon levels in houses with other substructure types may have decreased also, but the changes are not statistically significant.

The impact of weatherization on indoor air quality is rather modest with the exception of its impact on radon concentrations. In a house with a crawl space, the standard BPA weatherization package improves indoor air quality by reducing radon concentrations.

The findings from this study showed that indoor pollutant concentrations were low except for radon concentrations in existing houses in the Spokane area. The standard weatherization measures reduced the specific leakage area and therefore the ventilation in these houses by 12%. A poor correlation was seen between ventilation changes and changes in pollutant concentrations. Finally, weatherization had a modest effect on pollutant concentrations other than radon. Weatherization caused radon concentrations to decrease significantly in crawl space houses.

Commercial Building Ventilation Measurements Using Multiple Tracer Gases*

William J. Fisk, Richard J. Prill, and Olli Seppanen

Indoor air quality and the efficiency of ventilation depend, in part, on the rate of supply of outside air and also on the spatial variability of ventilation and the indoor flow patterns. For example, some rooms may be over-ventilated and others under-ventilated. Another concern is the possibility that fresh air supplied at ceiling-level short circuits to ceiling-level return grills such that the occupied region is poorly ventilated. Such a flow pattern would be inefficient. Conversely, a displacement or piston-like flow pattern in the floor-to-ceiling direction would generally be efficient since the air exiting the building would typically have an above-average concentration of pollutants.

Three new parameters are used to describe the ventilation process in detail. The first parameter is the age of air which equals the amount of time the air has been in the building. The second parameter is the air exchange efficiency which equals the age of the air that exits the building divided by twice the spatial-average age of indoor air. The air exchange efficiency equals 0.5 when the indoor air is perfectly mixed--values below and above 0.5 indicate short circuiting and displacement flow patterns, respectively. The third parameter is the source of air fraction which equals the fraction of air at some location that entered the building through a particular air handler or by infiltration.

To measure these new parameters, we simultaneously label each incoming stream of outside air with a different tracer gas. Outside air may be labeled directly by injecting a tracer gas at a constant rate directly into the stream of outside air, or labeled indirectly by injecting the tracer into the mixture of outside air and recirculated indoor air. Tracer injection is continued until concentrations in the air exiting the building are stable. Using cart-mounted gas chromatographic systems, tracer gas concentrations are monitored versus time in the major ducts of the air han-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

dling units. During the period of injection, small local samplers in occupied spaces pump air/tracer samplers at a constant rate into one-liter sample bags yielding samples with time-average tracer concentrations. When tracer concentrations have stabilized, a syringe sample is collected at the location of each local sampler and operation of the local sampler is terminated.

Previously-established data analysis procedures based on age distribution theory have been modified to account for the use of multiple tracer gases. Source of air fractions are determined from ratios of steady-state tracer gas concentrations to measured (or predicted, if the outside air is labeled indirectly) concentrations of the same tracer gases in the streams of incoming outside air. Ages of air are determined from the source of air fractions and numerical integrations of the real-time tracer gas concentrations or by equivalent computations using the data collected at local samplers. Finally, the spatial average age of the indoor air is estimated by averaging the ages measured at numerous indoor locations.

The results of investigations in a complex of three interconnected office buildings and in an isolated office building are summarized. Within regions of these buildings that are served by a single air handler that supplies a mixture of outdoor and recirculated indoor air, the measured ages and source of air fractions varied by 30% or less from the region-average values. Monitoring at different heights above floor level provided no evidence of either short circuiting or displacement flow patterns within a room. Age of air varied more substantially between physically-isolated regions of a building (e.g., different floors with no mechanical recirculation between the floors) and between regions served by different air handlers. In the complex of buildings, air exchange efficiency values were close to 0.5, suggesting relatively uniform mixing of the indoor air in regions served by a single air handler. In the isolated building, air was supplied and removed from physically-isolated regions, and the air exchange efficiency was 0.7. Monitoring in additional buildings is required before general conclusions can be drawn regarding these aspects of ventilation in commercial buildings.

Indoor Exposure Assessment*

G.W. Traynor, A.V. Nero, S.R. Brown, M.A. Apte, and B.V. Smith

The Indoor Exposure Assessment Project has three major research themes: 1) to continue the development of a macromodel to characterize the frequency distribution of indoor pollutant concentrations; 2) to compile a data base of field measurements of indoor pollutants; and 3) to conduct assessments of the health risks associated with exposures to indoor air pollutants. Conceptually, the first two projects supply the data needed for the third project of assessing health risks from indoor air pollutants.

In FY 1988, modeling efforts assessing the distribution of indoor exposures to combustion pollutants were continued; the concentration of indoor pollutants (CIP) data base was expanded; and the overall assessment of carcinogenic risk from indoor exposures was advanced.

MACROMODEL TO ASSESS INDOOR CONCENTRATION DISTRIBUTIONS

A major effort of the Indoor Exposure Assessment Project has been to utilize available information on the behavior and occurrence of indoor pollutants as a basis for assessing, in a systematic way, the distribution of public exposures to important classes of indoor pollutants. Initial efforts of the project focussed on the problem of estimating exposures to combustion emissions. This effort has resulted in the development of a macromodel that can predict indoor pollutant distribution across houses for carbon monoxide (CO), nitrogen dioxide (NO_2) and respirable suspended particles (RSP).[1]

The model development was completed in FY 88. The model is based on, and is an expansion of, mass balance principles commonly used in IAQ studies. Keys to the model include the characterization of building stock parameters relevant to IAQ (e.g., house volume, air

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division, by the Assistant Secretary for environment, Safety and Health, Office of Environmental Analysis, and by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building System Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098; by the Directorate of Health Sciences of the U.S. Consumer Product Safety Commission through Interagency Agreement CPSC-IAG-86 with DOE; by the Gas Research Institute, Chicago, IL with DOE; and by the Electric Power Research Institute, Palo Alto, California through contract RP2034-14 with DOE.

exchange rate), the investigation of the market penetration of combustion appliances and other indoor combustion sources, and the development of source usage models. The model utilizes deterministic and Monte Carlo simulation techniques to combine all of the inputs yielding indoor pollutant concentration distributions.

Although the initial modeling efforts concentrate on three combustion pollutants, the model is being developed with explicit attention to future expansion of the model to describe other indoor air pollutants concentrations from a wide variety of sources.

The planned activities for FY 89 are: 1) finalize the formal report on the development of the model; 2) conduct sensitivity analyses and micro/macro comparisons of the model to rank information/modeling gaps; and 3) explore the potential for generalizing the model and expanding it to include combustion pollutants other than CO, NO_2, and RSP (e.g., polycyclic aromatic hydrocarbons, dinitropyrenes or other organic mutagens), radon, and non-combustion organic contaminants such as those arising from building materials, furniture, and consumer products.

CONCENTRATIONS OF INDOOR POLLUTANTS (CIP) DATA BASE

During the last ten years public and governmental concern regarding indoor air quality in this country and elsewhere has greatly increased. This concern has resulted in hundreds of field experiments being carried out to monitor pollutant concentrations and other relevant parameters in a wide variety of building types and geographic locations.

The goal of this project is to create a computerized data base of the results of field studies devoted to monitoring indoor air quality in occupied buildings in the United States and Canada.

A major update to the Data Base was prepared during FY 88. New bibliographic references, summary data sets were added. Several minor enhancements to the software were made.

Software was written to support user entry and editing of summary search data. When distributed, this would make it possible for the user to enter not only their own bibliographic data, but also summary data and text.

The first draft of a technical reference manual was prepared. This manual is designed to provide a journeyman programmer with enough information to modify and extend the data base system. It includes file specifications, heavily commented source code, a subroutine tree, and other useful information.

The CIP Data Base (Version 3.1) has been implemented in a microcomputer environment running MS-DOS, using dBase III, and a commercial dBase III compiler, Clipper.

Additional updates to the data base will be distributed during the fiscal year. The updates will include all available published work and final reports. In addition, the user community will continue to be supported. There are over 200 current users of the CIP Data Base.

RISK ASSESSMENT

The purpose of this work is to utilize exposure information as a basis for estimating the health risks due to various classes of indoor pollutants.

Earlier work in this area has made sufficient progress in examining risks of major pollutant classes that, together with other information, it is now possible to assemble tentative pictures of risk for certain health endpoints, at least for diseases like lung cancer, that are usually fatal.

The LBL effort has previously examined data on indoor radon concentrations as a basis for estimating the distribution of indoor concentrations, and hence exposures, in U.S. homes.[2] This indicates that the average indoor concentration is approximately 1.5 pCi/l (55 Bq/m^3) in single-family homes and that approximately 7% (or 4 million houses) have annual-average concentrations exceeding 4 pCi/l (150 Bq/m^3). Together with various epidemiological data, this leads to an estimate of the average lifetime risk of lung cancer due to radon exposures of about 0.4%,[3] with long-term occupants of houses with 150 Bq/m^3 incurring a risk exceeding 1% and those living at higher concentrations having proportionately higher risks.

This defines a spectrum of risk from radon that is much higher than the risks associated with typical environmental pollutants, i.e., those in outdoor air and in water supplies, and that compares with occupational risks or with risks associated with personal choices - e.g., accidents in homes or cars or, in the extreme, cigarette smoking. Similarly, analysis of organic chemicals indoors leads to an estimated average risk of cancer of 0.03-1% due to indoor exposures (depending on the form of dose-response model used).[4,5] This again is a large risk compared with other environmental situations.

This picture of risk of premature death due to indoor exposures can be filled out by noting the estimated effects of two other pollutants about which there has been much concern: environmental tobacco smoke (ETS) and asbestos.[6] Although controversial, midrange estimates of the risk of lung cancer to the average nonsmoker, due to breathing ETS, are comparable to the middle of the estimated range for organic chemicals just noted. Estimates of the risk from asbestos exposure, arising primarily indoors, are somewhat lower. Nonetheless, estimated risks from all of these indoor pollutants just named exceed 10^{-4}, which is larger than most environmental risks. This more complete, albeit tentative, picture of the risks of indoor pollutants provides a direct basis for considering the importance of indoor pollutants and influences the design of strategies to control indoor air pollution levels by contributing to fuller development of our general perspective on risks due to pollutant exposures.

We will continue to 1) reexamine radon risk estimates in the light of new data on U.S. radon concentrations and reanalysis of the full body of epideiological data, 2) undertake a general evaluation of our current state of knowledge on organic chemicals and their importance, and 3) include results from combustion exposure modeling in assessment of indoor risks.

REFERENCES

1. Traynor GW et al. Macromodel for assessing indoor concentrations of combustion generated pollutants: part I, model development and preliminary predictions for CO,NO_2 and respirable suspended particles. LBL-25211; 1988 (draft).
2. Nero AV, Schwehr MB, Nazaroff WW, and Revzan KL. Distribution of radon-222 concentrations in U.S. homes. 1986, *Science 234*:992.
3. Nero AV. Estimated risk of lung cancer from exposure to radon decay products in U.S. homes: a brief review. 1988, *Atmos. Environ.22:2205-2211.*
4. McCann J, Horn L, Girman J, and Nero AV. Potential risks from exposure to organic compounds in indoor air. 1986, LBL-22473.
5. McCann J, Horn L, Girman J, and Nero AV. Potential risks from exposure to organic carcinogens in indoor air. in Sanbhu SS, de Marini DM, Mass MJ, Moore MM and Mumford JS (Eds.). *Proceedings of EPA Symposium on Short-Term Bioassays in the Analysis of Complex Environmental Mixtures,* Durham, NC, October 20-23, 1986.
6. Nero AV. Elements of strategies for control of indoor air quality. *Indoor Air '87: Proceedings of the 4th International Conference on Indoor Air Quality and Climate: Volume 3,* Institute for Water, Soil and Air Hygiene, Berlin (West), pp. pp. 573-578.

Energy Performance of Buildings*

M.H. Sherman, R.C. Diamond, D.J. Dickerhoff, H.E. Feustel, M.K. Herrlin, A. Kovach, M.P. Modera, B.V. Smith, C. Stoker, and Y. Utsumi

The Energy Performance of Buildings Group (EPB) carries out fundamental research into the ways energy is expended to maintain desirable conditions inside buildings. Our results form the basis of design and construction guidelines for new buildings and retrofit strategies for existing buildings. In this article, the work carried out over the last year is split into four overlapping sections: 1) Existing Buildings Efficiency Research, 2) Air Infiltration, 3) Air Leakage, and 4) Wood Burning. The emphasis in our work is on whole building performance. We collect, model, and analyze detailed data on the energy performance of buildings, including the micro-climate, the building's thermal characteristics, the mechanical systems, and the behavior of the occupants. Because of the multidisciplinary approach we work closely with other groups, both at the Laboratory and elsewhere.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy and Office of Building and Community Systems, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, Idaho Department of Water Resources and the Bonneville Power Administration.

EXISTING BUILDINGS EFFICIENCY RESEARCH

As new buildings—both residential and commercial—are responding to higher energy prices and stricter energy codes by becoming more energy efficient, the existing stock represents a large untapped area for energy conservation activity. Of the three buildings sectors, single-family, multifamily, and commercial, multifamily has had the least level of activity, and presents some of the greatest challenges. Over one quarter of the U.S. housing stock is in multifamily buildings. The Office of Technology Assessment estimates that while current levels of retrofit activity in multifamily buildings are likely to save 0.3 quads of energy (320 petajoules) by the year 2000, the *potential* savings are more than three times as much.

The Existing Building Efficiency Research Program was initiated to address these problems in all three building sectors, single-family, multifamily, and commercial. The U.S. Department of Energy has designated LBL as the primary lab for carrying out research in the multifamily sector, and while the emphasis in the past years has been in coordinating research in this sector, we continue to work in single-family and commercial buildings. A review of the work in all three sectors is available.[1]

Protocol Development

The need for a standardized set of procedures for monitoring buildings has led to our developing a monitoring protocol for residential buildings. An earlier draft of the protocol was used to specify the monitoring procedures during field tests in multifamily buildings in Chicago and Minneapolis/St. Paul. The experience gained at these monitoring sites has been incorporated into subsequent drafts of the protocol. The objective of the protocol is to provide a comprehensive standard for data collection and evaluation of retrofit performance. A primary goal for the protocol work is the development of an ASTM and ASHRAE standard for building monitoring.

Development of Audits and New Diagnostic Techniques

While the protocol provides a guideline for long-term monitoring, practitioners and researchers also have a need for short-term diagnostic tests to understand the characteristics of the building shell and mechanical systems. In addition to having a tool box of basic diagnostic techniques, the practitioner needs a strategy for how to use them.

The *Multifamily Audit* currently under contract to Princeton University gives the necessary information for determining appropriate retrofits for an individual building.[2] Based on material developed by Princeton and LBL, the audit outlines the steps to evaluate, select, and analyze the performance of the retrofits in a multifamily building. A draft of the audit was prepared in conjunction with the joint Princeton/LBL diagnostic demonstration (March, 1988) and a final copy will be available by 1989.

Diagnostics for energy use in multifamily buildings that have been developed or are currently under development include tests of boiler efficiencies, distribution losses, shell and inter-apartment leakage, and household appliance efficiencies.

Following the development of air leakage diagnostics, we tested a ten-unit apartment building to determine air flows between units and to the outside. Results from these tests showed that the individual apartments were quite leaky to the outside, but had very little leakage between units, in contrast to the older buildings we had been studying previously.

Analysis of Retrofit Performance in Multifamily Buildings

We developed two models in the past year based on data collected from earlier monitoring projects in Chicago and Minneapolis. The first models the air flow through combustion appliances (i.e., heating and hot water systems) that exhaust through a common chimney, a situation that is typical in multifamily buildings. The model can be used to peredict the performance of retrofits such as vent dampers or flow restrictors based upon the physical configuration and operating characteristics of the system.[3]

The second model characterizes the seasonal efficiency of multifamily boilers, taking into consideration the venting issues described above, as well as jacket and ground heat losses. Jacket losses from the older brick-set boilers were as high as 12 percent. Newer, steel-case and sheet-metal boilers had jacket losses of 2-4 percent. More than 80% of the losses were found to occur in off-cycle. This model is capable of providing the data necessary to make recommendations for boiler retrofit or replacement.[4]

Institutional Barriers

The widespread adoption of many retrofits is hindered by institutional barriers, including split financial incentives between owners and tenants, lack of information on the part of building managers, and a wide range of behavioral issues. We evaluated three projects this year that looked at institutional barriers, the first on the role of apartment managers in determining the energy use in multifamily buildings, a second study on how to improve information about energy use and savings to homeowners and renters based on their utility bills, and a third project that looked at how decisions are made that affect the energy use in new office buildings.

The study of apartment managers surveyed several groups and building organizations that have addressed the problems of improving energy efficiency in multifamily buildings through better operations and maintenance. Motivation and feedback were found to be the two key elements in ensuring adequate attention by the building managers. We undertook case studies to examine the basic problems confronting apartment managers, and innovative solutions to these problems were documented.[5]

One of the difficulties in retrofit research is finding simple ways to evaluate the performance of the retrofits. Often the only feedback available to homeowners who have undertaken retrofits is to compare utility bills from before and after the retrofit. While energy researchers can weather-normalize the pre- and post-retrofit energy consumption, homeowners will typically compare only their costs, receiving potentially misleading information.

In work carried out by the Center for Environmental Studies, Princeton University, we collaborated on a project to provide a sample of households in New Jersey with a home energy report which showed their monthly household energy consumption, weather-normalized, for a two-year period. The households were then surveyed to determine whether they found this information useful, whether it helped them determine if their previous retrofits were successful, and whether the information would encourage them to take further steps in conserving energy. The results of this feedback study showed that while most households appreciated having the information, and found it quite interesting, many were unable to grasp the concept of weather normalization. Several of the households, however, thought that the information would help them keep track of how much energy they were using.[6] In 1988 we started a similar study to focus on providing information to tenants in multifamily buildings.

We completed the evaluation of two innovative office buildings designed to showcase new energy technologies. The work was carried out in collaboration with Princeton University, and focused on the design process and how decisions affecting energy performance were made. As part of the study we evaluated the tenants' satisfaction with the buildings.[7] An off-shoot of this work will be our involvement in FY '89 in evaluating a sample of new energy-efficient buildings in the Pacific Northwest.

AIR INFILTRATION AND VENTILATION

With improved insulation of the building shell, heat loss from ventilation—whether controlled or by infiltration—has become an even more important fraction of a building's overall heat loss. Our air infiltration and ventilation work is split into three areas, multizone modeling, ventilation and moisture analysis, and support for the International Energy Agency's ventilation annexes.

Multizone Modeling

A number of computer programs have been developed to calculate air flow patterns in buildings. Awareness of the airflow pattern in a building is particularly important when (1) determining indoor air quality for the different zones in a building, (2) evaluating smoke distribution during a fire, and (3) calculating space conditioning loads. Sizing space conditioning equipment is also dependent upon accurate air flow information.

To treat the true complexity of the air flows in a multizone building, extensive information is needed regarding flow characteristics and pressure distributions both inside and outside the building.[8] To reduce the input data required by detailed infiltration models, simplified models have been developed. Most of these, including the one

developed at LBL, simulate infiltration associated with single-zone structures.

A high percentage of existing buildings, however, have floor plans that characterize them more accurately as multizone structures. Although multizone models exist, the vast majority are not readily available to the end user.[9] These models need inordinate amounts of input data. Therefore, a simplified multizone model capable of providing the same accuracy as the established single-cell models is being developed at LBL.[10]

The first validation of the simplified model for predicting multizone air flows was completed this year.[11] We plan to validate the model in the coming year through multigas tracer measurements both in the laboratory and in the field, as well as through an extensive collaborative international effort with the *Laboratoire d'Energie Solaire (LESO)* at the Ecole Polytechnique Federale de Lausanne in Switzerland.

The bulk of the multizone infiltration modeling work was done in cooperation with the Joint Research Centre of the European Communities in Ispra, Italy. Work included the preparation for the COMIS workshop in FY89. COMIS (Conjunction of Multizone Infiltration Specialists) is a year-long international workshop scheduled to take place at LBL during FY89. Experts from approximately 10 different countries will work together to complete the problem of predictive modeling of air flow in multizone buildings. The intended outcome is a general purpose computer code for use by designers, policy makers, researchers, etc.

Ventilation and Moisture

The MultiTracer Measurement System (MTMS) is a multigas tracer system that allows the simultaneous determination of the air flows between all of the zones within a building, as well as to the outside. The system is built around a quadrapole mass spectrometer which allows fast measurement of the concentration of all the tracer gasses in all zones. Injection of the tracer gas is controlled to keep a nearly constant concentration of the tracer in the zone it is injected. This is done to optimize the measurements and is not required for the analysis, as is the case in a single-gas system. MTMS has been used to measure up to five zones within a building and has the capability to measure eight.

This year MTMS was used in a comparison between multi-zone measurement systems developed by LBL, Princeton University and Brookhaven National Lab.[12] Of the three systems, MTMS gave both the greatest information about air flows and had the most flexibility.

Figure 1 shows a three day segment of one of the trace gases (gas 3) in fize zones of the apartment complex. Zone 1 is an upstairs apartment and has no connection to the other zones. Zone 4 is a district heat exchanger room and has a large exhaust fan. At time 75.6 the door between zone 3 and 4 is closed and we see the concentration of gas 3 increase in zone 3 and decrease in zone 4. To obtain the desired target concentration of 10 ppm (of

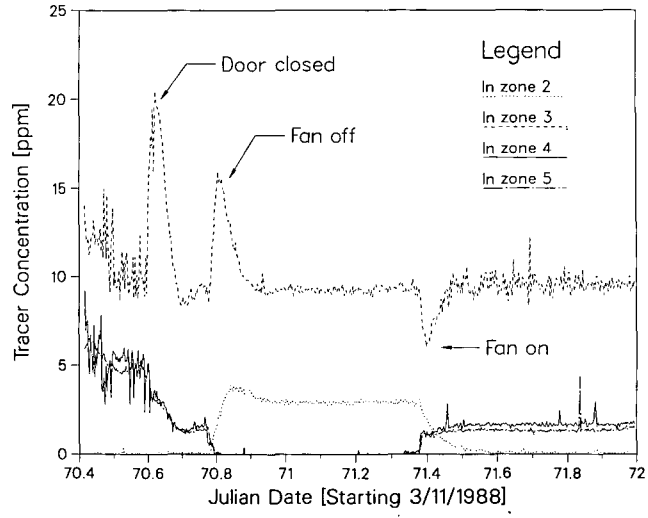


Figure 1. Tracer gas concentrations in a four-zone configuration. Controlled concentration is in the zone 3.

gas 3 in zone 3) the injection rate is reduced. A similar response is seen at 70.8 when the exhaust fan is turned off, and its opposite at 71.4 when the fan is turned back on.

MTMS was also used in Princeton to measure air flows in conjunction with measurements on radon levels in a residence which used either electric resistance or central forced air heating systems.[13] The information MTMS provided about inside air flows and flows in combustion devices helped to determine radon entry behavior and flow paths. MTMS was also used in two residences in the Pacific Northwest as part of a study to compare blower-door and passive ventilation measurement techniques.

Our effective ventilation efforts have provided techniques for estimating how much passive ventilation measurement techniques will underestimate the average ventilation rate. For typical housing the underestimates are at the 20% level. Results of the air flow calculations for the data set shown in Figure 1 are given in Figure 2. Note the large drop in flows when the door is closed and when the exhaust fan is turned off. We can also see that the flow direction between zone 3 and 2 changes when the exhaust fan is turned off. Estimated errors for these flows are typically about 10% for flows to/from outside and 20% between zones.

In FY 88, we also initiated a field monitoring project in College Station, Texas to examine the performance of a ventilation strategy for hot, humid climates. The strategy being examined consists of using pressurization ventilation in conjunction with a heat-pump water heater in the cooling season, and exhaust ventilation with the same heat pump during the heating season. This strategy should provide cost-effective ventilation and moisture management, as well as hot water, during the summer, while providing the conventional benefits of exhaust ventilation with heat recovery in the winter. Long-term data acquisition sys-

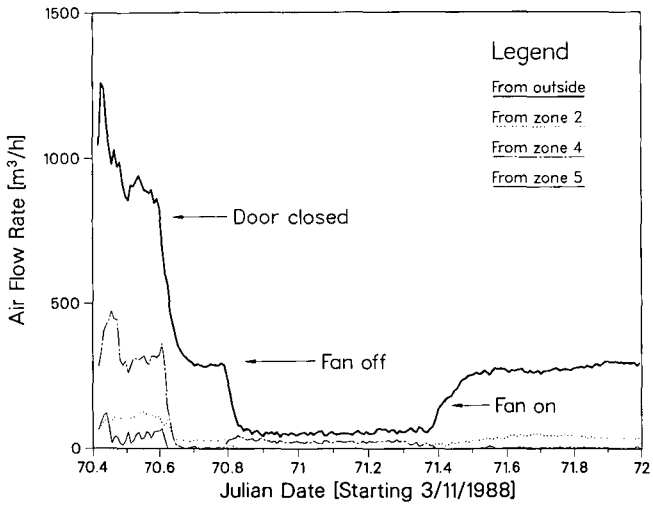


Figure 2. Air flows calculated from data in Figure 1 showing influence of fan operation and door openings.

tems were installed in both houses this summer, and the ventilation systems installed in both houses in the fall. The systems will be monitored continuously for the next year, including flip-flop tests between the systems and conventional electric resistance heating.

International Energy Agency (IEA) Support

In response to the 1973-74 oil crisis, the OECD countries formed the International Energy Agency. As part of the implementation agreement, technical annexes were created to enable countries to work together on problems of mutual interest. To date, twenty technical annexes have been formed. As the U.S. representative to Annex V, the Air Infiltration and Ventilation Centre, we provide interested parties with information material, e.g., the quarterly published Air Infiltration Review, which is sent to over 640 U.S. researchers and professionals. We also distribute the AIVC Technical Notes to interested parties. During FY 88 the Air Infiltration and Ventilation Centre responded to over 100 inquiries from the U.S. and delivered over 600 copies of technical papers held in their library of some 2,200 ventilation-related papers.

AIR LEAKAGE

The process of air flowing through unintentional apertures is called air leakage. In buildings, air leakage occurs through apertures in the building envelope, in mechanical systems, and in between building zones. Air leakage flowrates depend both on the air tightness of the building component as well as on the pressures driving the flow. For building envelopes, the technique used for measuring and characterizing their air tightness, the fan pressurization technique has evolved over the past ten years. The air tightness of residential-building mechanical systems (e.g., central furnace ducts) and the air tightness of internal partitions between zones (e.g., in multifamily buildings) have only recently begun to be examined.

Our air leakage research can be divided into three areas: leakage characterization, measurement techniques, and consensus standards. Our leakage characterization effort involves collecting and analyzing measured leakage data, as well as understanding the fluid dynamics of air leakage. As part of our measurement technique research we have developed alternative techniques for measuring building envelope airtightness, including AC Pressurization and Pulse Pressurization, and are presently developing techniques for measuring the air leakage in residential duct systems and multi-zone buildings. Finally, we are putting our experience to use by assisting the professional societies in the formation of consensus standards.

Air leakage research efforts in FY 88 focused on measurement technique development and analysis, specifically on the development of the Pulse Pressurization technique for measuring single-zone leakage, an analysis of the effects of wind on fan pressurization measurements, and on the development and analysis of multi-zone leakage measurement techniques.

The Pulse Pressurization technique determines the leakage characteristics of the envelope of an enclosure (e.g., building) from the decay of the building pressure from an elevated value down to its steady-state value.[14] During FY88, the theoretical work needed to extract the leakage characteristics of the envelope from the pressure decay was performed, as was an experimental examination of the technique in a small test structure.[15,16] The robustness of the technique was tested using the experimental data obtained, this analysis indicating that although loss mechanisms other than leakage can affect the decay of the oscillating components of the pressure, the technique provides repeatable measurements of envelope air leakage. These results imply that future implementations of the pressure-impulse mechanism will be designed so as not to excite the normal modes of the structure or its contents, which is accomplished by simply increasing the rise-time of the pressure impulse.

As fan pressurization involves the measurement of the fan flows required to maintain measured indoor-outdoor pressure differences, wind-induced pressure variations add uncertainty to the measurement. During FY88 we performed a theoretical analysis of the effects of wind on fan pressurization measurements, as well as an analysis of experimental data taken in at the University of Alberta to explore the these effects. The results of these analyses indicate that wind-induced measurement uncertainties can be significantly attenuated using a four-wall pressure averaging probe and time-block averaging of pressure and flow data. The analyses also demonstrated a wind-induced bias in leakage area measurements for both single-pressure and four-wall-average pressure techniques.

As part of our work with professional committees and organizations, we were involved with two standards-writing organizations: the American Society for Testing and Materials (ASTM) and the American Society of Heating Refrigeration and Air-conditioning Engineers

(ASHRAE). We participated in several activities in ASTM during FY 88, including the modification of Standard Test Method E-779, "Determining Air Leakage Rate by Fan Pressurization" and related standards. We are also involved with ASHRAE standard project 119P, which is intended to promote energy conservation by setting maximum values for air leakage in detached single-family residential buildings. After a five year effort this standard was approved by ASHRAE.

Air leakage research efforts in FY 89 will focus on further development of the Pulse Pressurization technique, further testing of AC-pressurization and fan-pressurization techniques for measuring inter-zonal leakage, and analysis of existing data on residential duct leakage. The multi-zone techniques will tested under controlled conditions in a multi-zone building. The duct leakage analysis will be based on data in our air-leakage database, data taken over the past several years by our staff, and on data taken as part of a field study performed by a monitoring contractor in Oregon.

The other focus of air leakage research in FY 89 will be in leakage characterization. The objective of this work is to develop a workable physical model for air flow through large apertures submitted to dynamic pressure conditions. This more basic work has application both to our two dynamic leakage measurement techniques, AC pressurization and pulse pressurization, as well as to the dynamic flows associated with natural ventilation.[17]

WOOD BURNING

Approximately 14% of residential space heating in the U.S. is supplied by wood burning, which when added to industrial burning, adds up to more than 3% of our primary energy needs. More importantly, approximately one third of the primary energy needs of developing countries is provided by combustion of biomass. These factors, along with the fact that wood and other biomass combustion typically occurs at very low efficiencies with high emissions of noxious gasses, particulates and greenhouse gases, have been the impetus behind the wood-burning research in our group. Our work has included the development of techniques to measure the thermal efficiency of wood burning in the laboratory and in the field, as well as studies of emissions from wood burning.

Based upon a single-channel woodstove heat-output monitor we developed several years ago, a study of wood heat delivery to single family residences was conducted in the Pacific Northwest. In FY 88, in collaboration with Pacific Power and Light, we continued our comparison between measured wood stove heat outputs and reported wood use based upon occupant surveys and site visits.[18] The principal finding of this study was that the apparent field efficiencies of wood burning averaged between 20% and 30%, far below the quoted laboratory efficiencies of 40% to 60% for the types of stoves monitored. Based upon these findings, and on the apparent changes in efficiency over the course of the two-year study, it seems clear that the conventional technique for estimating wood energy delivery is both imprecise and biased. This can be explained either by concluding that field efficiencies are far below laboratory ratings and thus the laboratory procedure should be reexamined, or by concluding that occupant reported wood use, even in conjunction with site visits by trained technicians is both a biased and uncertain estimator of actual wood consumption.

The other accomplishment in wood-burning research in FY 88 was the completion of a study of the effects of wood load and wood surface area on emissions from wood burning.[19] This study provided a simple theoretical explanation for trends in emissions found in experiments performed at the Royal Institute of Technology in Sweden. Based upon the oxygen-controlled nature of enclosed wood burning, it was shown that emissions of CO, CH_x, and soot scaled almost linearly with the amount of wood surface area above some critical value (dependent upon the rate of air supply). The results of this study have implications for wood-burning policy, stove design, and appropriate test methods. In FY 89, we hope to expand our capabilities to include the development of appropriate test methods for the efficiency and emissions from cookstoves in developing countries.

REFERENCES

1. MacDonald JM, Karnitz MA, Diamond RC, Ritschard RL, Mixon WR, Sherman MH. Research update: existing building efficiency research, 1987-1988. ORNL/CON-268, Oak Ridge National Laboratory, 1988.
2. Dutt GS, Harrje DT. Multifamily building energy audit procedure, interim version. Princeton University, 1988.
3. Dumortier D, Modera MP. A model for predicting air flow through venting systems for multiple combustion applications. Lawrence Berkeley Laboratory Report LBL-23151, 1988.
4. Modera MP. Jacket and stack losses from multifamily boilers. *Proceedings of the 1988 American Council for an Energy Efficient Economy Summer Study*, Asilomar, California, 1988.
5. Diamond RC. Building managers: hidden actors in multifamily energy conservation. *Home Energy*, Vol. 5, No. 2, 1988.
6. Layne LL, Kempton W, Behrens A, Diamond RC, Fels M, Reynolds C. Design criteria for a consumer energy report: a pilot field study. PU/CEES Report No. 220, Princeton University, 1988.
7. Diamond RC. Enerplex revisited: a post-occupancy evaluation. PU/CEES Report No. 222, 1988.
8. Kula HG, Feustel HE. Review of wind pressure distribution as input data for infiltration models. Lawrence Berkeley Laboratory Report LBL-23886, 1988.
9. Feustel HE, Kendon VM. Infiltration models for multicellular structures: a literature review. Lawrence Berkeley Laboratory Report LBL-17588, 1985.
10. Feustel HE, Scartezzini JL. (draft) Development and validation of a simplified multizone infiltration

model. Lawrence Berkeley Laboratory Report LBL-23036, 1989.

11. Haugen T, Feustel HE. Applications of a simplified model for predicting air flows in multizone structures. Presented at the 8th AIVC Conference on Ventilation Technology-Research and Application, Uberlingen, Federal Republic of Germany. Lawrence Berkeley Laboratory Report LBL-23035, 1988.
12. Harrje DT, Dietz RN, Sherman MH, Bohac DL, D'Ottavio TW, Dickerhoff DJ. Tracer gas measurement systems compared in multifamily and commercial buildings. Princeton University, Center for Energy and Environmental Studies, 1988.
13. Hubbard LM, Bolker B, Socolow R, Dickerhoff DJ. Radon dynamics in a house alternately by forced air and by electric eesistance. Princeton University, Center for Energy and Environmental Studies, 1988.
14. Yuill GK. Method and apparatus for testing the air tightness of a building using transient pressurization. United States Patent No. 4,510,791, 1985.
15. Sherman MH, Modera MP. Signal attenuation due to cavity leakage. *Journal of the Acoustical Society of America 84*, December 1988, Lawrence Berkeley Laboratory Report LBL-24289, 1988.
16. Bonnefous Y. Pulse pressurization - a technique for measuring building air leakage. Ecole Nationale des Travaux Publics de l'Etat, Lyon, France, 1988.
17. Modera MP, Sherman MH, and Vacheron PF. Pulse pressurization: a technique for measuring building air leakage. September 1987, LBID-1321.
18. Yoder R, Modera MP, Spolek G. In-situ wood heat monitoring: evaluation of Measured heat output and field efficiency. *ASHRAE Trans.* 94(I): 1988.
19. Modera MP, Peterson F. Reducing emissions from wood stoves by reducing wood surface area. Lawrence Berkeley Laboratory Report LBL-22910, 1988.

PUBLICATIONS LIST

Indoor Radon

LBL-24179
"Parametric Modeling of Temporal Variations in Radon Concentrations in Homes" K.L. Revzan, B.H. Turk, J. Harrison, A.V. Nero, R.G. Nero R.G. Sextro. 2fIEEE Transactions on Nuclear Science, vol. 35, no. 1, pp.550-555 (1988).

LBL-24344
"Mapping Surficial Radium Content as a Partial Indicator of Radon Concentrations in U.S. Houses," K.L. Revzan, A.V. Nero, R.G. Sextro (1988).

LBL-24345
"Appraisal of the U.S. Data on Indoor Radon Concentrations, " A.V. Nero, K.L. Revzan, R.G. Sextro (1988).

LBL-25127
"Evaluation of Radon Reduction Techniques in Fourteen Basement Houses: Preliminary Results, " B.H. Turk, et al. *Proceedings of the 81st Annual Meeting of the Air Pollution Control Association*, Dallas, TX, June 19-24, 1988, Paper No. 88-107.2, APCA, Pittsburgh, PA, May 1988.

LBL-25292
"Radon Entry and Control in Seven Homes with Basements," R.G. Sextro, B.H. Turk, J. Harrison, K.L. Revzan, A.V. Nero, (1988).

LBL-25762
"Predicting the Rate of Radon-222 Entry from Soil into the Basement of a Dwelling due to Pressure-Driven Air Flow," W.W. Nazaroff (1988).

LBL-25910
"Intensive Radon Mitigation Research: Lessons Learned," B.H. Turk, R.J. Prill, R.G. Sextro, J. Harrison (1988).

Indoor Organic Chemistry

LBL-25465
"Evaluation of Soil-Gas Transport of Organic Chemicals into Residential Buildings: Final Report," A.T. Hodgson, K. Garbesi, R.G. Sextro, J.M. Daisey, (1988).

LBL-24964
"Efficiencies of Portable Air Cleaners for Removal of Nitrogen Dioxide and Volatile Organic Compounds," J.M. Daisey, A.T. Hodgson, *Proceedings of the 81st Annual Meeting of the Air Pollution Control Association*, Paper No. 88-111.4, Dallas, TX (1988).

LBL-25519
"Experiments and Modeling of the Soil-Gas transport of Volatile Organic Compounds into a Residential Basement," K. Garbesi, (1988).

Indoor Air Quality and Controls

LBL-22315
"Indoor Air Quality and Ventilation Measurements in 38 Pacific Northwest Commercial Buildings Volume 1: Measurement Results and Interpretation, and Volume 2" B.H. Turk, et al. (1988).

LBL-23135
"Commercial Building Ventilation Rates and Particle Concentration," B.H. Turk, et al. (1988).

LBL-23451
"Exhaust-Air Heat Pump Study: Experimental Results and Update of Regional Assessment for the Pacific Northwest," P.H. Wallman, W.J. Fisk, D.T. Grimsrud, (1988).

LBL-23979
"Pacific Northwest Existing Home Indoor Air Quality Survey and Weatherization Sensitivity Study," B.H. Turk, et al. (1988).

LBL-25614
"Commercial Building Ventilation measurements Using Multiple Tracer Gases," W.J. Fisk, R.J. Prill, O. Seppanen, (1988).

LBL-25718
"The Impact of Gas Furnace Operation in Radon Concentrations in Residences: A Literature Survey," D.T. Grimsrud, D.M. Odenwalder, (1988).

Indoor Exposure Assessment

LBL-22473
"Potential Risks from Exposure to Organic Compounds in Indoor Air," J. McCann, L. Horn, J. Girman, A.V. Nero, (1988).

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
1 CYCLOTRON ROAD
BERKELEY, CALIFORNIA 94720