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SOLAR ENERGY PROGRAM CHAPTER

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APPLIED SCIENCE DIVISION ANNUAL REPORT SOLAR ENERGY PROGRAM FY 1984

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SOLAR ENERGY PROGRAM

INTRODUCTION

During FY 1984, the Solar Energy Program at Lawrence Berkeley Laboratory (LBL) continued to focus on research extending the technology base for a broad range of solar energy applications and to explore new approaches to solar energy conversion.

Passive approaches to heating, cooling, and lighting of buildings are a major research topic. In these technologies, architectural design, construction materials, and natural energy flows between the interior and exterior environment are used to control a building's interior climate and reduce consumption of nonrenewable energy. In FY 1984, LBL examined the application of passive solar technologies to commercial buildings. Projects in both systems development and materials research were carried out.

In commercial buildings, cooling and lighting requirements typically dominate energy operating costs. For this reason, research in passive systems development was directed at daylighting and passive cooling. These activities were supported by system simulations, heat transfer research, and performance monitoring and evaluation.

In the daylighting project, a facility for measuring illumination levels and light quality in scale models of buildings was used to generate a data base on the illumination performance of roof aperture systems. These data were in turn used in building energy analyses to examine the total energy impacts of various roof aperture configurations in office buildings. In addition, a comprehensive evaluation of the effectiveness of roof apertures in two existing nonresidential buildings was completed. This evaluation examined not only the energy benefits of daylighting but also the functional and aesthetic advantages of daylit spaces and attempted to trace the energy benefits to their sources in the technology and in the occupants' response to it.

In passive cooling research, heat transfer studies with the long-term goal of quantifying the effectiveness of ventilation cooling strategies were conducted. These studies consisted of numerical modeling of convection processes to characterize the convection coefficients between ventilation air and building surfaces—especially for thermally massive constructions. Previous analyses of laminar convection in enclosures were extended to turbulent flow conditions, such as would be experienced with most forced ventilation cooling systems.

In a second project, theoretical analyses determined the extent to which the effectiveness of thermal storage materials in buildings is affected by the magnitude of the convection coefficient coupling the storage material to the air in the building. This project demonstrated that, in many passive heating and cooling systems, the known variability of the convection coefficients is large enough to substantially influence overall building performance and that efforts to describe this variability in terms of the physical parameters of the system are therefore warranted.

Systems analyses in FY 1984 investigated the total energy impacts of advanced aperture materials in daylit office buildings. Such materials provide control of the transmissivity of the aperture, thereby controlling solar heating and illumination of the occupied space. These advanced materials would allow oversizing of building apertures to minimize lighting electricity requirements without adversely impacting cooling energy requirements. A comprehensive examination of the effect of structural thermal mass on heating and cooling energy requirements for residential buildings was also carried out. Finally, in conjunction with the American Institute of Architects Foundation, we began a study of energy requirements and passive opportunities in educational buildings. Such buildings constitute one of the major nonresidential building types for which substantial passive opportunities are expected to exist.

Research on advanced aperture materials also continued. This work is intended to identify and develop promising new optical materials for the next generation of high-performance glazings. Research focuses on four technical areas:

(1) Low-conductance, high-transmittance materials; e.g., durable low-emittance glazings and transparent aerogels.
(2) Optical-switching materials; e.g., electrochromic coatings.
(3) Angle-selective transmitting materials.
(4) Materials to enhance daylight utilization in buildings; e.g., light-guide systems.

The research includes technology assessment studies and multiyear research planning; materials synthesis; studies of optical, thermal, chemical, and structural characteristics; stability and durability studies; energy performance studies; and activities to transfer results of our work to appropriate industrial and other private-sector users.

LBL is also engaged in research on the active solar cooling of buildings. Thermodynamic cycles that have the potential for increasing the efficiency of solar-driven absorption air conditioners by at least a factor of 2, compared to the current state of the art, are being studied. An air conditioner based on one of these advanced cycles, the double-effect regenerative absorption cycle, was tested, modified, and retested throughout FY 1984. Stable and efficient operation has been achieved, with near-design performance. In parallel with the experimental work, simulations and analyses of solar cooling systems have been performed to establish the operating requirements and thermal performance of current and advanced space conditioning systems. This work is helping to determine future research needs for the DOE solar cooling program. Activities in FY 1984 concentrated on the effects of storage-control and chiller-control strategies on solar cooling system performance.

Installation of a 25-ton-capacity solar absorption air conditioning system in LBL Building 71 as part of the Solar in Federal Buildings Program will afford LBL engineers the opportunity to gain first-hand experience with one of the new solar cooling units developed in the DOE solar R&D program. The solar collectors and a water-deionization system for the collector loop were installed during FY 1984. Operational testing will start early in FY 1985.

In both active solar cooling and passive solar, LBL staff has provided technical support to DOE Headquarters and the DOE San Francisco and Chicago Operations Offices in developing program plans, evaluating reports and proposals, and technical monitoring of R&D activities by other contractors.

Research continues to explore advanced concepts for using the microstructural properties of materials in conversion, control, and collection of sunlight. The goal is to find and develop solar applications for small-particle suspensions, aggregates, and diffractive structures through a balanced program of experimental and analytical studies. Previous successful solar testing of the Small Particle Heat Exchange Receiver (SPHER) has led to new research efforts to investigate direct radiant heating of particle suspensions for chemical process applications, for thermal energy storage, and for the detoxification of chemical wastes.

In related research, LBL is developing new materials formed from aggregates of small particles (aerogels), both for transparent insulating windows and as intermediate states in the fabrication of ceramic materials with superior properties.

Finally, one of our more basic research projects concerns biological energy conversion techniques, using one of the simplest and most stable biological energy converters known: the pigmented protein bacteriorhodopsin. This project is attempting to elucidate how the molecular structure of this protein uses sunlight to produce an electrical proton current across bacterial and artificial membranes. Such understanding should ultimately suggest ways to produce novel photoelectric cells and solar batteries.

Passive Solar Research and Development*

R.C. Kammerud, J.W. Place, M.R. Martin, M. Adegran, H. Akbari, P. Albrand, B. Andersson, F.S. Bauman, P.H. Berdahl, W.L. Carroll, J.P. Coutier, A. Mertol, J.T. Thornton, and T. Webster

The amount of conventional fuel used to heat, cool, and light buildings is determined by (1) the interaction of the building with its environment, (2) the thermal gains associated with the activities occurring within the structure, (3) the thermal storage characteristics of the building, and (4) the operating characteristics of the equipment used to convert conventional fuels to end-use energy. Traditionally, the building design process has not adequately accounted for the combined influence of these four factors on building energy consumption. To do so requires that the designer have access to techniques for properly controlling the interactions of the building with its environment and for managing the energy flow within the structure.

Passive heating, cooling, and lighting strategies integrate energy control and management schemes into the building design. The design parameters are selected so that they enhance and control the coupling of the building to the environment, thereby reducing the requirements for auxiliary heating, cooling, and lighting energy. In this context, the Passive Solar Program at Lawrence Berkeley Laboratory is directed at theoretical and experimental investigations of the energy performance implications of passive design strategies, with emphases on passive and hybrid cooling and natural lighting of commercial buildings. The specific objectives of the program are to:

(1) Develop analytic descriptions of the energy processes that occur within a building and between a building and its environment.
(2) Develop and evaluate advanced passive/radiative cooling systems.
(3) Evaluate the effectiveness of passive systems in reducing energy consumption for space heating, space cooling, and lighting.

*This research was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Solar Heat Technologies, Passive and Hybrid Solar Energy Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The strategy to meet these objectives consists of coordinated experimental and theoretical tasks leading to advanced energy analysis capabilities for passive system design and evaluation. The emphasis has been on the development and testing of techniques for predicting both the "resource" for passive systems and a building's response to that resource. Here the term "resource" implies the naturally occurring potentials of the environment to provide heating, lighting, and cooling. These potentials are being investigated in projects on convection, radiative cooling, natural lighting, and passive building energy analysis. Accomplishments and plans in each of these topics are described below.

ACCOMPLISHMENTS DURING FY 1984

Ventilation Cooling

Two ventilation cooling projects were completed during FY 1984, both addressing the cooling of nonresidential buildings. In the first project, a 10,000-ft^2 single-story office building was modeled, using the BLAST† building energy analysis computer program to determine the cooling energy savings attainable through night ventilation. Four perimeter zones and one core zone were served by a single heating, ventilation, and air-conditioning (HVAC) system and a parallel fan system capable of flushing the interior space at either a low speed (3 air changes per hour) or a high speed (up to 30 ach). Electricity consumed by the fans was included in the total building energy budget for cooling.

Computer simulations were carried out for three climates: New York, Los Angeles, and Atlanta. It was found that increasing the building's internal mass, even without night ventilation, reduced its cooling energy requirements by up to 10% in all three climates. Los Angeles had the greatest benefit from night ventilation. Energy savings can be larger in the winter if the 30-ach system is used; in summer, the lowest energy use is achieved with the lower flow rate.

The second ventilation project consisted of modeling a two-story, 20,000-ft^2 office building having a hollow-core concrete floor between the two levels. Night ventilation air is flushed through the core spaces, which are modeled as "minizones" in BLAST. This system was modeled for the climates of New York and Los Angeles. The results indicated

†BLAST (Building Loads Analysis and System Thermodynamics) is trademarked by the Construction Engineering Research Laboratory, U.S. Department of the Army, Champaign, Illinois.

that heat transfer between the occupied spaces occurs with adequate efficiency by thermal conduction through the slab. Recirculation of air between the slab and the occupied spaces does not result in further performance improvements. Reductions in cooling energy were less than 10% in both climates. Best results were obtained with a ventilation rate of 12,000 cfm through the 10,000-ft^2 slab for 7 to 10 hours each night.

Energy Use in Educational Buildings

This project is part of a large, comprehensive study being conducted by the American Institute of Architects Foundation (AIAF) for DOE. The overall objective is to gain knowledge about the number of buildings, actual energy consumption, and opportunities for solar applications in nonresidential buildings. The objective of the FY 1984 effort, of which the LBL work is a part, is to demonstrate the efficacy of a methodology for gaining this knowledge by applying it to one building category, and specifically to demonstrate methods by which:

(1) The number of buildings in the most important nonresidential building categories can be determined.
(2) The key energy characteristics can be identified.
(3) The actual energy use of a category of buildings can be estimated.
(4) The present and future opportunities for solar applications can be assessed in terms of potential energy savings and cost benefits.

Schools were chosen as the example building category to demonstrate the methodology because:

- Schools are the third largest energy consumer among all categories of nonresidential buildings.
- Office buildings have already been extensively analyzed.
- Retail buildings are difficult to prototype.
- A relatively large body of data is already available and can be used without requiring major new efforts.
- A moderate increase in school enrollment is projected for the rest of the decade.

The LBL work for FY 1984 consisted of systems analysis in support of goal (4) i.e., to analyze key energy factors for the school building category. One school prototype was analyzed with the BLAST program to determine building boundary energy consumption and the effect of variations in envelope and HVAC system operating characteristics. Identification and assessment of various solar applications will be the focus of future work. The prototype building specified by AIAF was a 125,325-ft^2, three-story concrete block building with an enrollment capacity of 1000 pupils. The prototype model included a variety of functional spaces typical of actual schools. These functional areas were agglomerated into the following major categories: kitchen, cafeteria, gymnasium, auditorium, shops, classrooms and administration offices, and restrooms. The kitchen specifications were determined from a detailed analysis of typical menus and equipment with the assistance of a dietitian. The building was arranged as a "T" structure so that orientation effects could be identified. The operating schedules included holidays and summer vacations as well as a summer session. Cooling equipment was specified for all functional areas except the restrooms, shops, gymnasium, and kitchen.

Simulations were performed for the baseline configuration in three climates: Los Angeles, New York, and Atlanta. The results are summarized in Figs. 1–3. In addition, the following parametric runs were made in all three climates to identify key energy issues and possible savings:

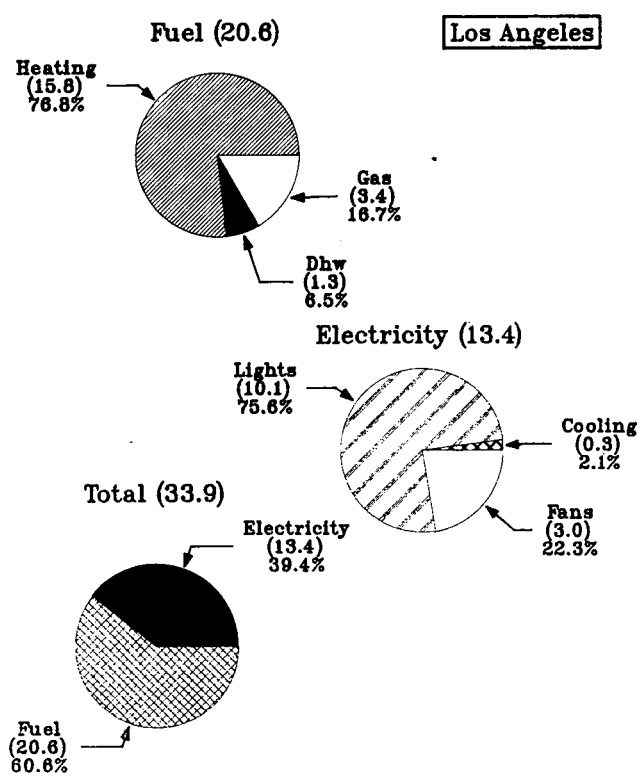

Figure 1. Annual building boundary energy consumption (kBtu/ft^2) for Los Angeles climate. (XBL 854-1946)

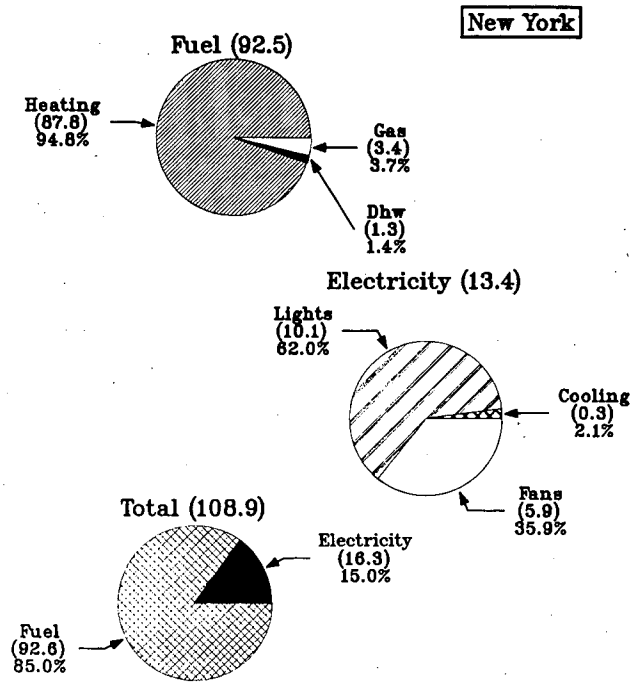

Figure 2. Annual building boundary energy consumption (kBtu/ft^2) for New York climate. (XBL 854-1948)

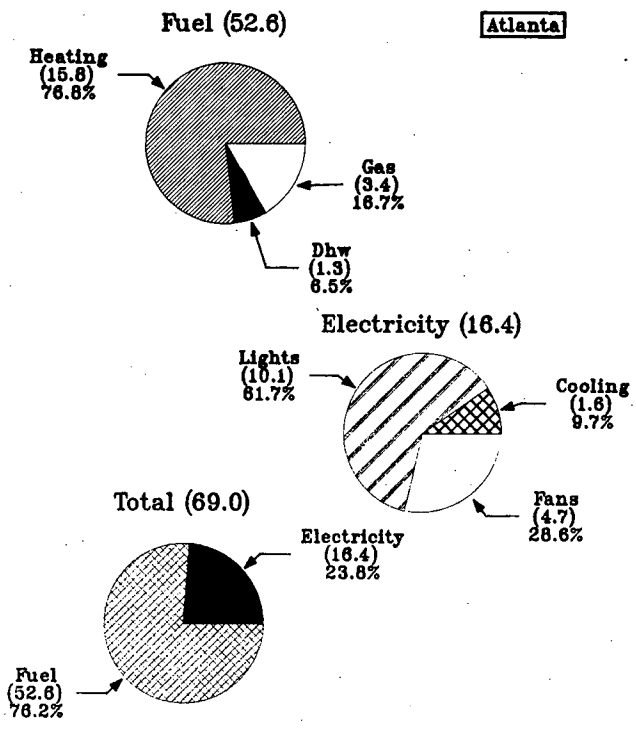

Figure 3. Annual building boundary energy consumption (kBtu/ft^2) for Atlanta climate. (XBL 854-1947)

- *Infiltration*—the baseline infiltration rate was reduced by half.
- *Ventilation*—the outside air ventilation rate through the HVAC equipment was reduced by approximately 17% (this reduction in outside air is equivalent to the infiltration reduction).
- *Solar gains*—the window transmission was reduced by 50% to determine the effect of differences in solar gains.
- *Wall conductance*—the R value of the opaque walls was increased by 22% to determine the effect of adding insulation to the walls.

The results of these parametric runs are shown in Figs. 4–6.

Experimental Buildings

Twenty-three passive commercial buildings have been designed and built with DOE support.[1] These are experimental buildings that push state-of-the-art design by incorporating advanced conservation features and passive heating, cooling, and lighting strategies. The buildings are being used to examine

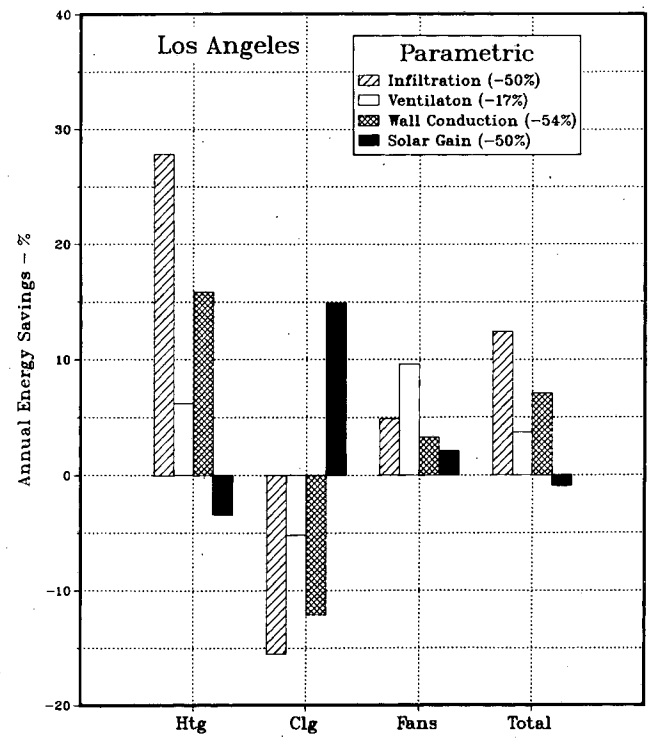

Figure 4. Annual energy savings (%) for four building parameters, Los Angeles climate. (XBL 854-1952)

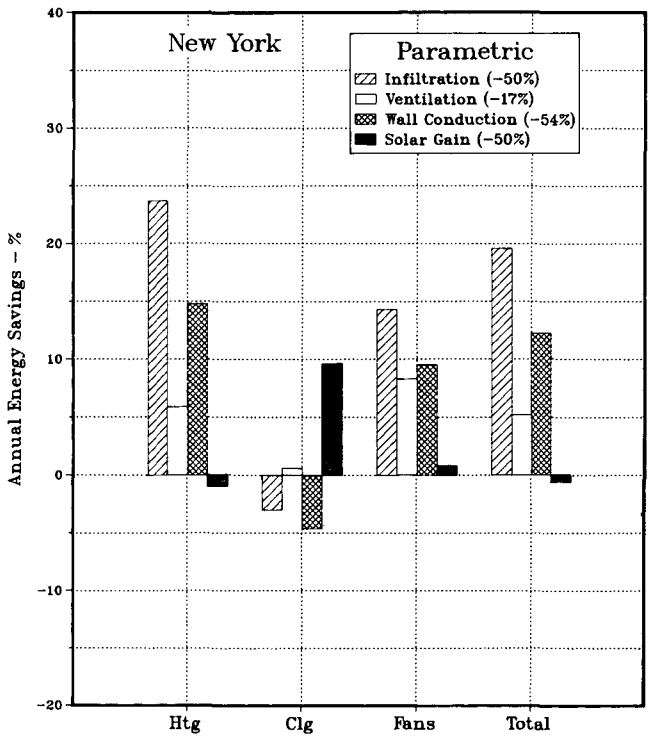

Figure 5. Annual energy savings (%) for four building parameters, New York climate. (XBL 854-1951)

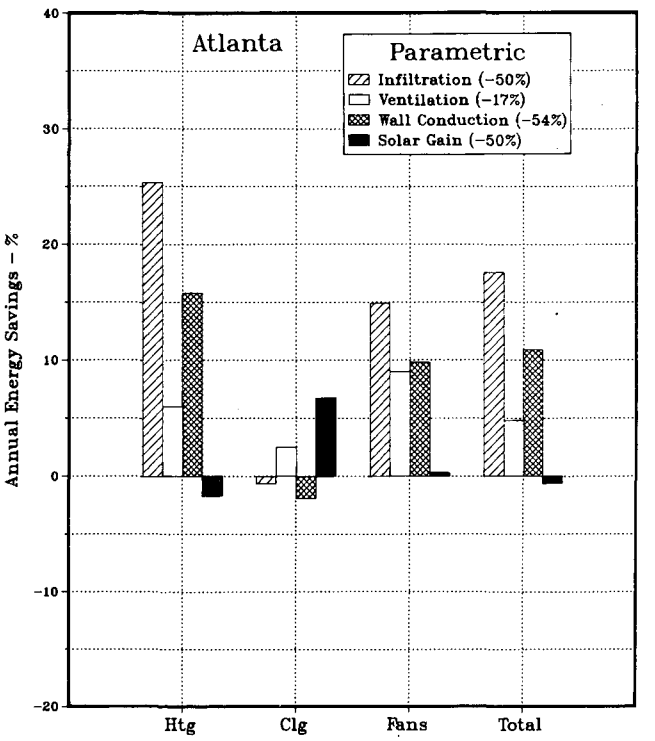

Figure 6. Annual energy savings (%) for four building parameters, Atlanta climate. (XBL 854-1950)

the effectiveness of these passive strategies in commercial buildings, thereby better defining research needs in heat transfer, modeling, analysis, and design. The information gathered directly from these buildings is also valuable for confirming or providing a basis for modifying the occupancy and energy-related assumptions typically made during the design process.

The passive commercial experimental buildings program has entered the performance evaluation phase, in which studies are being made of (1) occupancy effects on thermal performance and occupant satisfaction and (2) thermal and energy performance. Data have been collected on the design process and the designs themselves. In addition, performance data have been collected for a 12-month period after occupation; this consists of reports on occupancy schedules and occupant satisfaction as well as energy-use data. In some projects, specialized automated monitoring and data acquisition systems have recorded hourly data.

As part of this large national program, the Passive Solar Research and Development Group is conducting the *Extended Analysis Project*, which consists of two subprojects: (1) analysis of the effect of roof monitors on lighting, heating, and cooling, with special consideration given to lighting control strategies, both manual and automatic; and (2) analysis of the thermal effects resulting from variation in occupancy and occupant interaction with passive systems. The major effort in FY 1984 has been to complete the first project and establish the parameters for the second.

The roof monitor analysis is of particular interest because roof monitors play a major role in the passive systems of 80% of the experimental buildings. The study has provided considerable information to direct future research in a field that is still identifying the basic potentials of different daylighting approaches.

Figure 7 illustrates the method used in this effort for analyzing lighting control strategies, a method so far applied to two sites. The many discrepancies that are possible when comparing the actual building and the computer simulation are eliminated by running BLAST simulations in all cases. The only difference is the manner in which the lighting schedule input is generated; the rest of the building description is identical. Results have shown that occupant control of electric lighting can be a viable strategy for both energy use and lighting sufficiency.[1]

Thermal analysis of other issues related to occu-

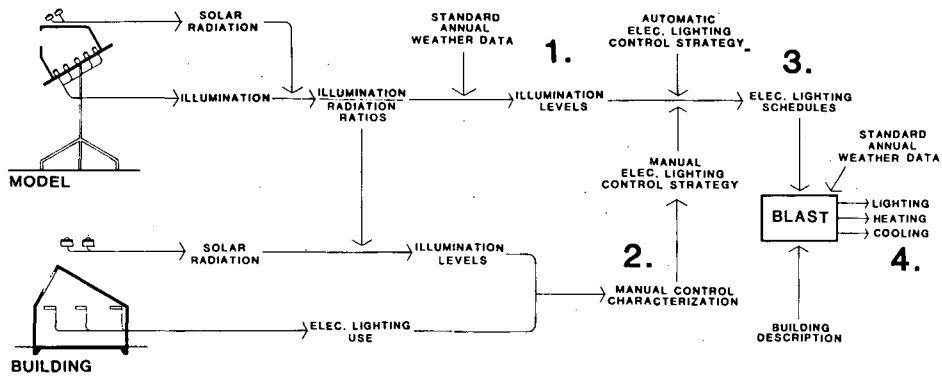

Figure 7. Methodology for analyzing lighting control strategies, showing how BLAST will compare a model and an actual building. (XBL 854-1941)

pant comfort, satisfaction, and interaction with passive systems draws on the work of Min Kantrowitz, an LBL subcontractor. Kantrowitz identified the following important occupant-related issues: (1) *thermal mass*—the sensitivity of energy use and comfort to mass amount and exposure; (2) *thermostat setback*—its integration with mass and effect on comfort; (3) *acoustics*—its impact on energy use and competition with passive systems for surface area; and (4) *shading*—energy-use sensitivity to variations in shading and shade control. BLAST will be used to simulate alternatives in each of these areas. Several buildings from the experimental program will be simulated to provide a range of situations for each topic.

Natural Lighting

In FY 1984, energy analyses were performed on a prototypical, single-story office building outfitted with a variety of roof apertures. The emphasis was on assessing the effect of roof glazing area, orientation, and tilt in moderating the interaction of the building with the solar resource. To assess the implications of this moderating process, calculations were made of lighting electricity consumption, cooling electricity consumption, heating fuel consumption, peak electricity demand, and annual energy operating costs for the building in a range of U.S. climates. The following combinations of orientation and tilt were examined:

- horizontal;
- south-facing vertical;
- south-facing tilted up 60° from the horizontal;
- north-facing vertical;
- north-facing tilted up 45° from the horizontal;
- combined south- and north-facing verticals;
- combined east- and west-facing, both tilted up 60° from the horizontal;
- combined southeast- and southwest-facing, both vertical;
- combined southeast- and southwest-facing, both tilted up 60° from the horizontal;
- combined north-, south-, east-, and west-facing, all vertical;
- and combined northeast-, northwest-, southeast-, and southwest-facing, all vertical.

For each of these glazing orientations and tilts, simulations were performed for a range of roof glazing areas between 0% and 10% of the building floor area, except for north-facing vertical glazing, where the weak collection of sunlight indicated the need to examine larger glazing areas.

Figure 8 shows the results of some of these simulations for linear roof apertures on a prototypical office building in Atlanta, Georgia. For weather conditions, Typical Meteorological Year (TMY) data were used.

In Fig. 8(a), annual lighting electricity consumption (at the site) is plotted against the aperture ratio, defined as the ratio of total roof glazing area to building floor area. (The consumption of primary energy by the utility to generate power would be three to four times higher than consumption at the site, because of generating inefficiencies and electrical network losses.) The four curves correspond to roof glazing with the following orientations: vertical facing south, vertical facing north, vertical facing both south and north (equally divided), and horizontal (skylights). At all aperture ratios, horizontal glazing has the lowest lighting electricity consumption,

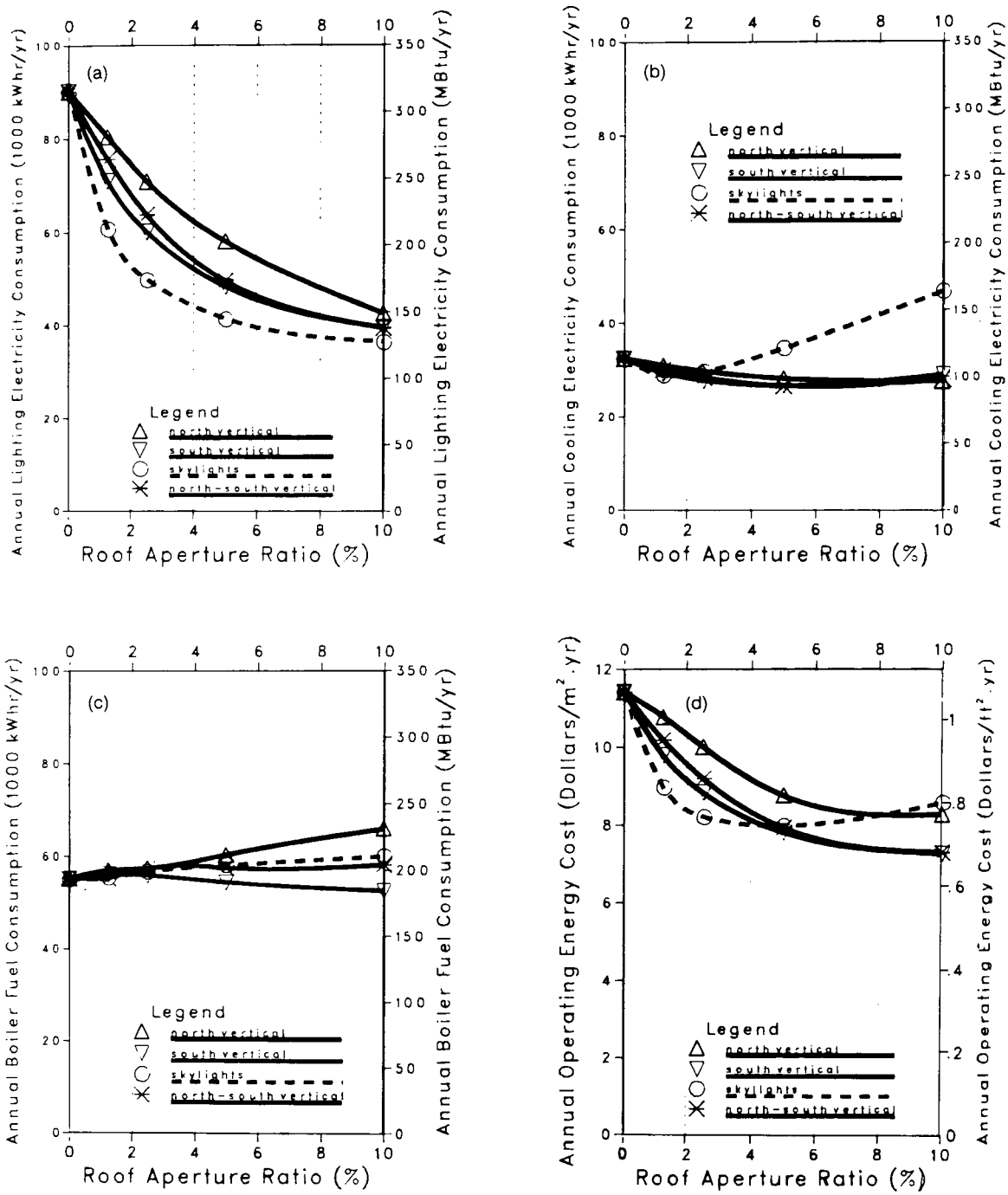

Figure 8. Results of simulations of linear roof apertures on a prototype office building in Atlanta, Georgia, showing the effect of roof aperture ratio on annual energy consumption and cost. Typical Meteorological Year Data were used. (a) Lighting electricity consumption; (b) cooling electricity consumption; (c) boiler fuel consumption; and (d) operating energy cost. (XBL 848-3318A)

reflecting the highly effective annual collection of both diffuse skylight and beam sunlight. The north-facing glazing, on the other hand, has the highest lighting electricity consumption at all ratios, reflecting the negligible collection of beam sunlight and the weaker collection of diffuse skylight (vertical glazing

faces only half the skydome). About halfway between these two curves is the curve for south-facing glazing. Vertical glazing facing south collects substantially more beam sunlight than vertical glazing facing north but is substantially less effective than horizontal glazing in the annual collection of both diffuse skylight and beam sunlight. If lighting electricity reductions were the only impact of roof apertures, then horizontal glazing would clearly be the preferred glazing orientation. However, the thermal impacts of roof apertures are also important.

Figure 8(b) plots annual cooling electricity consumption at the site (fans plus a direct-expansion cooling unit) against aperture ratio. For small aperture ratios, the cooling electricity consumption decreases as the ratio increases because all the admitted sunlight is being used to displace electric light of higher heat content. In fact, at small ratios (around 1%), the glazing orientations that collect most effectively during the cooling season have the lowest cooling electricity consumption, i.e., horizontal glazing has the lowest lighting electricity consumption and vertical north-facing the highest. At larger aperture ratios, the order of the curves is reversed, in the sense that the glazing orientations that collect most effectively during the cooling season produce the highest cooling electricity consumption. This is because, at larger aperture ratios, solar gains frequently exceed the illumination requirements of the building. These excess gains create a thermal load that is not offset by reductions in heat from unused electric lights. In general, the cooling electricity consumption curves suggest that horizontal is not the preferred orientation for roof glazing, contrary to the results for lighting electricity consumption.

In Fig. 8(c), boiler fuel consumption is plotted as a function of aperture ratio. In general, the curves tend to be fairly flat. Also, the cost per unit of heating fuel energy at the site is substantially lower than the corresponding cost of electrical energy. Economically, therefore, the variations in boiler-fuel consumption with aperture ratio are relatively inconsequential.

Finally, Fig. 8(d) plots the annual operating energy cost cost—the combined results of (a), (b), and (c)—as a function of aperture ratio. When the ratio is small but increasing, all curves decrease. The rate of decrease in the operating energy cost is largest for the glazings that collect sunlight most effectively. At larger ratios, however, the cost curve for horizontal glazing levels off and then starts to increase. This is because increases in cooling energy consumption and summertime peak demand offset the decrease in lighting electricity consumption. For all vertical glazings, the costs continue to decrease with increasing aperture ratio up to the full 10%. However, all three curves for vertical glazing are essentially level at the 10% ratio, suggesting that there is little benefit in going to larger ratios for this particular building type, glazing material, and electric lighting control system.

We may summarize all these results as follows:

(1) For small apertures, horizontal glazing yields the greatest cost benefit.
(2) For larger glazing areas, vertical glazing facing south or both south and north yields the greatest cost benefit.
(3) Vertical glazings facing south or both south and north also produce the largest cost benefit per unit of building floor area.
(4) Horizontal glazing produces the largest cost benefit per unit of installed glazing area.

In general, the results indicate substantial potential benefits from fairly small glazing areas. For example, at a 2% aperture ratio, horizontal glazing produces an annual energy operating cost savings of about $20 per square foot of glazing.

In addition to the parametric analysis of glazing area, orientation, and tilt, simulations were also performed to determine the sensitivity of the energy and cost predictions to various assumptions in the analysis. Among the factors examined were: thermal comfort conditions in the building, more sophisticated thermal controls, glazing characteristics, obstruction of daylight by snow and dirt, and various internal surface treatments.

Of particular significance was the detailed examination of thermal conditions in the prototype building. This study suggested that air temperature alone is not an adequate indicator of thermal comfort in buildings that aggressively use environmental resources to reduce energy consumption. In order to deal with nonuniform thermal environments, the Passive Solar Research and Development Group has added a detailed thermal comfort analysis subroutine to BLAST, thereby facilitating a more accurate assessment of the thermal performance of passive buildings.

Design integration studies were initiated in FY 1984. The emphasis was on using the analysis results in a design process examining the integration of the roof apertures with other building systems, such as the building structure, electric lighting, interior design, the HVAC system, and other passive strategies. Concepts were generated for a variety of roof configurations, both lightweight and thermally massive. A folded-plate wooden structure was stu-

died in detail (Fig. 9). At a lower level of effort, a study was conducted on a device for projecting beam sunlight into multistory buildings.

Residential Thermal Mass

LBL is carrying out a residential thermal-mass analysis project that has two major phases: (1) a validation phase in which simulation predictions are compared with measured data collected by other participants in the program and (2) a parametric simulation phase in which predictions of the effects of various thermal mass configurations in models intended to represent realistic buildings will be developed and analyzed. The first phase has been completed, and its results are described here.

The project uses energy performance simulations based on the BLAST-3.0 computer program. BLAST is a comprehensive energy analysis simulation tool that employs a detailed heat-balance solution method with an hourly time increment that correctly accounts for the effects of structural thermal mass on the dynamics of building energy consumption.

The work completed this year consisted of detailed hourly comparisons between measured data and BLAST predictions for three physical parameters: space loads, air and wall surface temperatures, and wall heat fluxes. Comparisons were made over several 10-day periods for three test cells at two experimental field sites operated by the New Mexico Energy Research and Development Institute (NMERDI) and the U.S. National Bureau of Standards (NBS).

The comparison involved development of BLAST inputs describing each cell in detail, based on plans, drawings, and other detailed descriptions from the experimentalists who constructed them. These inputs were coupled with weather files developed from measured on-site data for each location and all time periods, and hourly simulations of the test cells were performed. The predicted performance was compared with the measured data for 10 parameters in the three categories mentioned above: heating or cooling loads, as appropriate; air and wall surface temperatures for all four walls of the test cells; and heat fluxes for each wall.

A statistical analysis of the hourly predicted and measured values of these parameters was made. In general, the results show good agreement, varying from the 10% range for loads to the 20% range for the more detailed parameters such as wall heat fluxes. Additionally, the hourly variations, as seen in time-series plots for all 10 parameters, show very good agreement; Figs. 10 and 11 show typical comparisons.

The net result of this work is to further verify the ability of BLAST to accurately predict energy performance, particularly in the case of varying amounts and types of thermal mass in the building envelope. This result provides the basis for the next phase of this project, the estimation of the effect of varying amounts of thermal mass in the envelopes of realistic residential building prototypes, using parametric simulation techniques. This phase will be completed in the next fiscal year.

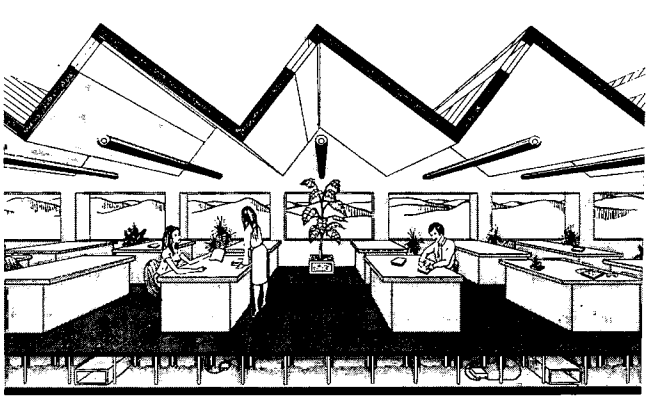

Figure 9. A linear roof-aperture system with diffusing glazing tilted toward the south. (XBL 854-1953)

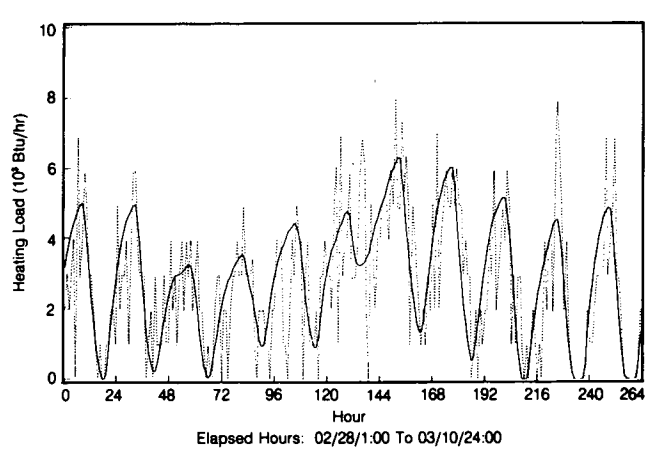

Figure 10. Comparison of measured and predicted hourly heating loads for a one-room test cell sited in New Mexico. The BLAST prediction is 5% higher than the measured data for the total load over the entire time period. (XBL 857-11644)

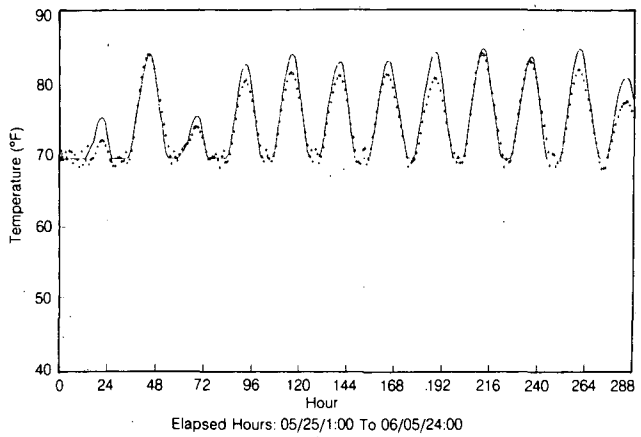

Figure 11. Comparison of measured and predicted hourly inside air temperatures for a one-room test cell sited in New Mexico. The BLAST prediction averages 0.7°F higher than the measured data over the comparison period. (XBL 857-11642)

Thermal Design Analysis for the UC Ten-Meter Telescope (TMT)

The University of California is designing and will build on top of Mauna Kea, Hawaii, a large (10-m) telescope using an innovative design.

Because of the potential for an enclosing observatory structure to adversely affect the seeing of the telescope, thermal effects associated with the structure are important to the design process. Generally, however, they have not been dealt with in detail in earlier observatory designs. The primary thermal design goal is to maintain all interior surface temperatures, particularly that of the mirror, at the exterior air temperature. The criteria for judging strategies to accomplish this are based on temperature differences between the outside air and the interior air and the telescope structure and mirror. The thermal design goals chosen for the TMT are nighttime root-mean-square (rms) temperature differences between outside air and various components, as follows: the interior air and all inside surfaces must agree to within 0.5°C; the front surface of the mirror, to within 0.25°C; and the back surface, to within 0.1°C of the front.

A series of computerized simulations of the observatory building and the enclosed telescope structure was performed to determine whether designs could be found that met the thermal goals stated above. A detailed description of the simulation model and its application and results are contained in a report in preparation.[2] We summarize the approach and its results here.

The simulation model used was developed for building energy research and simulates in detail the dynamic thermal performance of all building components. The simulation uses detailed descriptions of the structure geometry, materials, operating conditions, and external weather. Weather variables include air temperature, wind speeds, insolation, the effective temperature of infrared sky radiation, and ground temperature. By using a detailed heat-balance method, all heat flows and temperatures for each building component are determined hourly throughout the desired simulation period.

In the current application, the observatory dome, walls, and floor were all accounted for separately, as was the telescope structure, including the mirror itself. Weather conditions for several kinds of diurnal profile (typical, extreme, summer, winter) were determined from measured on-site data and used to drive the simulation. The thermal impacts of a number of observatory designs were determined by a systematic variation of several selected building design parameters, namely, insulation levels, surface radiation properties, operating schedules, and ventilation rates.

The results of these parametrized simulations clearly indicate that the overall thermal performance is controlled by a complex interaction between the thermal driving forces and the design parameters, and that changing one parameter has interactive effects with the others. However, we have also been able to identify a number of strategies that should yield a thermally optimal design, thus minimizing detrimental effects on seeing. These strategies are described below.

- *Building Insulation.* Insulating all interior surfaces of the observatory building is extremely important. Surfaces include the dome, the lower load-bearing wall, and the floor. For all surfaces, an insulation thickness of 10–15 cm is recommended. This will isolate the interior from conductive losses or gains due to external heat sources or sinks, such as daytime solar gains, infrared radiative heat losses to the sky, and the ground. It will also isolate the interior environment from the thermal mass of the various structural components. At night, the insulation will cause all surface temperatures to come closer to the outside air temperature—the basic thermal design goal.
- *Telescope Structure Insulation.* All telescope structural elements should be insulated with approximately 2–3 cm of standard industrial pipe insulation. This will cause the surface temperature of the structure to more closely

track the outside air temperature. In particular, it lessens the amount of stored heat that must be removed from the structure at the beginning of the nightly observing session.

- *Ventilation.* The observatory interior should be mechanically ventilated all night at a rate of about 10 volumetric air changes per hour. The ventilation should be started as early as several hours before sundown, whenever the outside air temperature is lower than the inside air temperature and heat removal can be accomplished. If observing continues after sunrise, ventilation should also continue.
- *Slit Control.* While avoiding direct solar gains, the slit should be opened about two hours before sundown. This will allow heat gained during the day to be dissipated. During the night, some fine-tuning of interior temperatures can be accomplished by controlling the area of the slit opening, consistent with viewing and weather protection needs.
- *Surface Infrared Emissivity.* All exterior and interior surface infrared emissivities should be high (0.9), except for the interior surface of the dome insulation, which should have a net effective emissivity of about 0.3. Since most normal building materials have an emissivity of about 0.9, only the dome interior surface needs special treatment. This recommendation eliminates bare aluminum as an undesirable exterior dome finish.
- *Dome Solar Absorptivity.* The solar absorptivity of the dome affects the net solar heat gain and thus has the potential for a significant impact on interior thermal conditions. Dome solar absorptivity should therefore be made as low as possible. A well-insulated dome, as recommended here, however, should decrease the negative impacts of solar gains.
- *Design Robustness.* Parametric variations involving weather data indicate that, while the thermal performance of the optimal design degrades somewhat with season and with different (and more extreme) diurnal patterns, this degradation is minor; the optimal design in fact appears to be relatively robust in such changes.

Figure 12 shows the thermal performance of two observatory designs—a "basic" one and an optimized variation—to compare how well the average

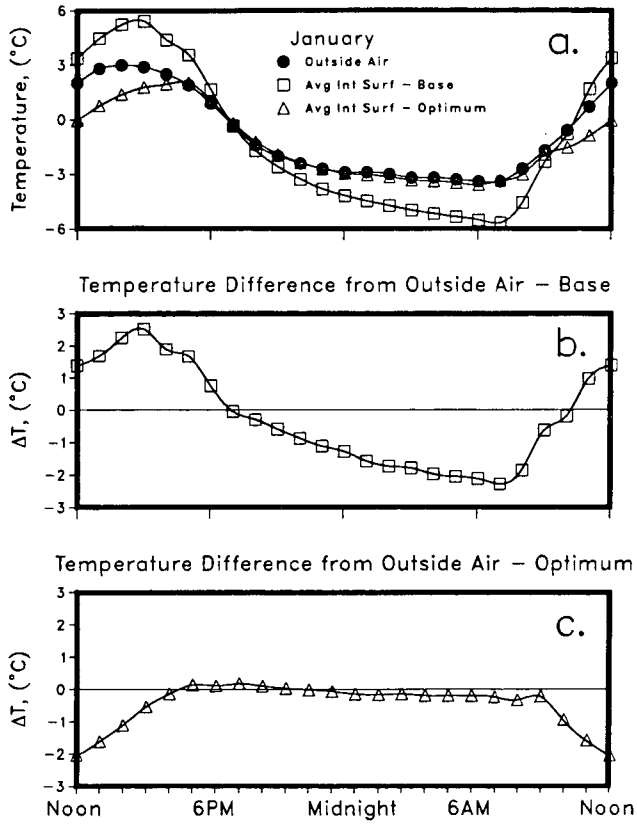

Figure 12. (a) Simulation results for "basic" and "optimal" observatory designs, comparing typical January external air temperatures and average interior surface temperatures; (b) average interior surface temperature for "basic" observatory design plotted as difference from external air temperature; and (c) average interior surface temperature for "optimal" observatory design plotted as difference from external air temperature. The time scale is in hours preceding or following midnight.

(XBL 854-1945)

inside surface and telescope structure temperatures for each design track the outside air temperature. It is clear that the optimal design tracks much better than the "basic" design, with rms nighttime differences of 0.17°C for the inside surface and 0.13°C for the telescope structure itself.

Thermal Comfort of Building Occupants

The importance of comfort problems in passive buildings is underlined by the growing feeling that total energy analysis of buildings should take into account occupants' response to their environment. One of these response problems is thermal comfort, of which we made a detailed analysis. (Other comfort issues include visual comfort, air quality, and acoustics.) Buildings using passive strategies typically

exhibit thermal nonuniformities, which have a significant impact on thermal sensations.

A detailed, state-of-the-art transient model predicting the human thermal response to a set of environmental conditions was selected and added to the simulation program BLAST. The input to the model consists of environmental variables such as air temperature, radiant temperature, solar flux (all calculated by BLAST for each hour and each thermal zone), air velocity, and relative humidity. Personal variables such as clothing and activity level are also input. The model's output is a matrix of comfort levels that can be analyzed statistically over the entire simulation period.

Figure 13 presents the results for a prototypical office building located in Atlanta, Georgia. Three strategies are compared in terms of their annualized impact on thermal comfort levels. Eight comfort bins (four on the cold side and four on the warm side) are defined to correspond to various comfort categories. The two middle bins correspond to the comfort region (as defined by having less than 10% of occupants dissatisfied). Compared to the baseline case, i.e., a building with reflective view glazings but no particular passive features, the two other strategies display thermal comfort implications that are notably different. The daylit building experiences mild warm discomfort for almost one-third of the time. This is caused by increased radiant temperatures and direct occupant exposure to solar radiation, both resulting from large solar apertures. On the other hand, the building with thermal mass and nighttime ventilation has some periods of cold discomfort, because of early morning exposure to cold radiant environments.

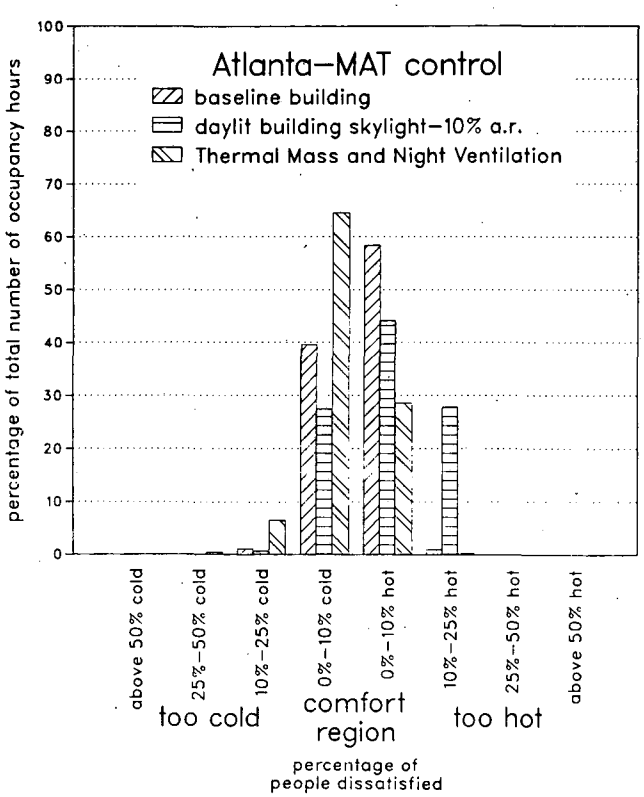

Figure 13. Analysis of thermal comfort conditions: a comparison of three passive strategies for a prototype office building in Atlanta, Georgia, as run on BLAST simulation program. (XBL 857-11643)

With this new tool, a new dimension has been added to the evaluation of potentials from passive options. Deeper analysis can now be made of tradeoffs between saving energy and meeting comfort criteria, particularly in daylit buildings and in buildings using advanced window materials.

Advanced Window Materials: Energy Impact of Variable-Transmission Glazings

We investigated the potential energy and cost savings of using variable-transmission glazings in a prototypical daylit office building with roof monitors. Simulations were performed on a developmental version of BLAST-3.0 to predict energy consumption and cost impacts. For a combination of climates, roof aperture areas, and electric lighting systems, we assessed the potential of optically "dimmable" glazing to reduce energy consumption associated with excessive solar gains through uncontrolled apertures.

The results indicated that, for large aperture areas (5% to 10% of the floor area), cooling benefits are substantial. This translates into operating cost savings ranging from $5 to $16 per year per square meter of controlled glazing in comparison with uncontrolled glazing ($0.45 to $1.50 per year per square foot), depending on climate, utility rate structure, and lighting design. Substantial benefits were also predicted for cooling system design costs and the thermal comfort of building occupants.

PLANNED ACTIVITIES FOR FY 1985

Energy Use in Educational Buildings

The objectives of this research in FY 1985 will be to identify the most promising passive strategies (both new and retrofit applications) for educational buildings and to examine the integration of the most promising of these systems into the design of these

buildings. To accomplish these objectives, LBL will conduct verification simulations of prototypical buildings, using actual building energy-use data available from the Tennessee Valley Authority. After the prototypes are "calibrated," simulations will be performed to identify key generic passive strategies and their energy savings potential. Once the most promising passive strategies are identified, design workshops will be conducted to determine design and cost implications for school buildings.

Experimental Buildings

Assessments of the importance of thermal issues related to occupant interactions with the building and of the sensitivity of energy use and comfort conditions to changes in building operation and configuration will be completed. LBL will contribute to the production of four comprehensive performance case studies and take major responsibility for producing two system studies that will coordinate results from several experimental buildings.

Natural Lighting

The natural lighting analyses performed on office buildings in FY 1984 will be extended to educational buildings. Design integration studies initiated in FY 1984 will continue. The emphasis in this work has been on using the analysis results in a design process that examines the integration of the roof apertures with other building systems, such as building structure, electric lighting, interior design, the HVAC system, and other passive strategies. At a lower level of effort, experiment and analysis will continue on a device for projecting beam sunlight into multistory buildings.

Residential Thermal Mass

Parametric energy simulations will be performed on a realistic residential prototype in a range of climates to estimate the effect of various amounts of thermal mass in the envelope. We will attempt to develop correlations between the predicted mass effect and building and climate parameters.

Thermal Design Analysis for the UC Ten-Meter Telescope

The focus will be on simulating and optimizing strategies for temperature control of the telescope mirror in the optimal dome environment that we have now identified. Pending additional funding, we would like to extend this work to cover design recommendations for improving the thermal performance of existing observatory facilities by retrofitting; we would also like to strengthen the simulation-based conclusions by direct measurement of some of the quantities used as input assumptions.

REFERENCES

1. Andersson, B. *et al.* (1985), *Effect of Daylighting Options on the Performance of Two Existing Passive Commercial Buildings,* LBL-18069.
2. Carroll, W.L. and Connor, C. (1985), *Thermal Modeling of the Dome*, TMT Report No. 134, Keck Observatory Science Office, Lawrence Berkeley Laboratory (forthcoming).

Optical Materials Studies*

S. Selkowitz, A.J. Hunt, C. Lampert, M. Rubin, and P. Tewari

Significant reductions in energy consumed by the building sector will come not only from better building design strategies but also from the development and introduction of new glazing materials. Since the inception of our program in 1976, identification, characterization, and exploratory development of promising new fenestration materials have been major activities. Research on new optical materials and on modifications of existing glazing materials is intended to create a technology base to assist industry with developing the next generation of advanced fenestration systems.

In addition to the research projects described in the following sections, the overall Optical Materials effort at LBL includes development of a multiyear research plan and scientific coordination of related DOE-funded research projects at universities, private sector firms, and other national laboratories. Results of the DOE-supported program are made available to interested parties in the private sector. For example, an annual technical conference and industry forum is held each year in August in conjunction with a meeting of the International Society for Optical Engineering (SPIE). This meeting serves as a forum to review and discuss the direction of the overall DOE program as well as to report on recent technical progress. A joint international effort on glazing optical materials under the auspices of the International Energy Agency is being developed with our participation.

In 1976, when our program began, we identified the development of low-emittance ("low-E") coatings as a major program objective. DOE-supported research activities have helped the fenestration industry to accelerate market introduction of new high-performance window systems incorporating these coatings. Several small firms began offering commercial products in 1982, and in 1984 many of the largest glass and window manufacturers introduced "low-E" products. In the near term, the use of low-E coatings in a conventional double-glazed window provides better thermal performance than triple glazing and makes a lighter and more compact window. In the long term, this coating technology offers the potential to produce transparent windows having heat transfer values as low as those of insulating walls. On an annual basis, such windows should outperform the best-insulated wall, even for a north orientation in a cold climate, since diffuse solar gain will offset some conductive losses. We initiated planning in late 1984 for a Low-E Window Roundtable, to be co-sponsored with the National Fenestration Council. We believe that the positive impact of this DOE-supported effort can serve as a model for the transfer and development of research findings in other optical materials areas.

GLASS AND PLASTIC SUBSTRATES

Accomplishments During FY 1984

To predict the optical properties of complex window systems incorporating thin-film coatings, the optical properties of the glass and plastic substrates must be accurately known. These properties have not been available in a complete and self-consistent form even for the most common varieties of glass used in windows, hence the need for this measurement effort. This year, we completed work on standard clear glasses, glasses having absorbing additives, and high-purity glasses. Our results are summarized in a paper that includes a complete set of optical constants from the near ultraviolet through the little-studied far infrared for all common window glasses.[1] We also provide some spectrally and directionally averaged bulk properties for calculating solar and thermal radiative heat transfer through windows. Figure 1 shows the real and imaginary components of the complex index of refraction for a clear glass as determined by Kramers-Kronig analysis of reflection measured with a Fourier-transform spectrometer over the near-infrared and infrared spectrum.

Future measurements will be greatly simplified with our new spectrometer, which covers the ultraviolet to the near infrared. In addition to having optics that are far superior to those of our previous instrument, this system features completely automated operation and data collection. The instrument is installed and operating, although not all functions have been tested.

Planned Activities for FY 1985

We will collect, organize, and catalogue our low-emissivity samples. These samples will be com-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division; the Office of Solar Heat Technologies, Passive and Hybrid Solar Energy Division; and the Office of Energy Systems Research, Energy Conversion and Utilization Technology Program of the U.S. Department of Energy under Contract No. DE-ACO3-76SF00098.

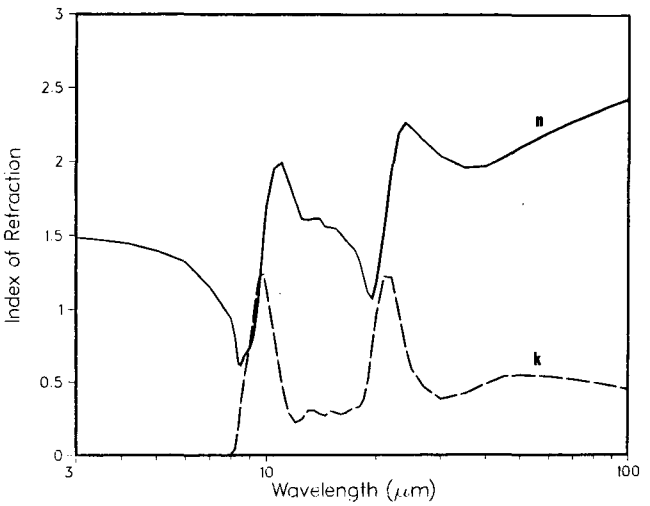

Figure 1. Real (n) and imaginary (k) parts of the complex index of refraction for soda-lime silica glass.
(XBL 8412-5271)

pletely characterized as part of our participation in the Low-E Window Roundtable in August 1985. Our spectrometer will be fully functioning.

LOW-CONDUCTANCE, HIGH-TRANSMITTANCE GLAZINGS

An ideal glazing material for residences in cold climates would have good optical clarity, high solar transmittance to admit sunlight in winter, and low thermal conductance to reduce heating costs. Such windows would perform better than insulated walls on an annual basis, even in northern orientations in cold climates. Simulation results for a north-facing window in Madison, Wisconsin are shown in Fig. 2. Windows must have U-value and shading coefficient combinations that place them to the right of the "0" net heat transfer line if they are to provide net energy benefits. Two promising research activities are under way to develop the technical basis for such advanced windows.

LOW-EMITTANCE, GRADIENT-INDEX COATINGS

Accomplishments During FY 1984

Since 1976, we have contributed to the development of window coatings that transmit sunlight but reflect in the thermal infrared, thus suppressing radiative heat transfer. Commercially available coatings based on metal-dielectric multilayer films have satisfactory optical properties but are not sufficiently durable to be used in nonsealed glazings. By producing a film having a continuously varying index of refraction to reduce reflection in the solar spectrum, we could use materials that are inherently more durable but less transparent than the metal films. Our analytical studies suggest that a gradient-index coating could improve solar transmittance by 25% without reducing emittance or durability.

We have begun by studying the titanium oxynitride (TiN_xO_y) system, producing these gradient-index coatings by plasma-assisted chemical vapor deposition (CVD). Better compositional control and durability have been achieved in a limited number of samples deposited by magnetron sputtering. We installed a new sputtering system and completed the first tests for homogeneous coatings. The coatings are being characterized by electron microscopy, Auger electron spectroscopy (AES), and Rutherford backscattering (RBS), in addition to complete optical

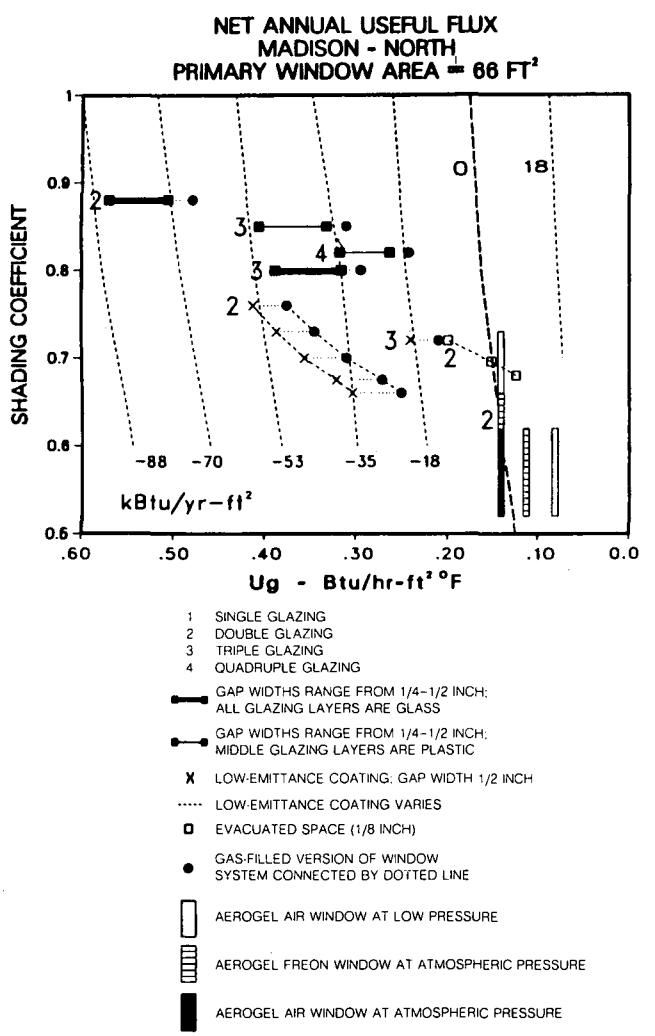

Figure 2. Simulation results for north zone, Madison, Wisconsin. (XBL 856-2870)

characterization. RBS has proven particularly valuable in our efforts to remove impurities from the coatings. Figure 3 shows the small amount of chlorine remaining in the coating after adding H_2 to scavenge the bulk of the unwanted Cl in our CVD films.

Planned Activities for FY 1985

We will add reactive gas-handling capabilities to our sputtering system to produce TiN_xO_y films. The process parameters will be varied in an attempt to achieve the optimum optical properties predicted by our analytical models.

AEROGELS

An unusual material, silica aerogel, is being developed at LBL for application as a transparent insulating window.[2,3] Aerogel is a microporous silica material containing a high fraction of voids (up to 97% by volume). It is transparent rather than translucent because the pore size is much smaller than the wavelength of light; therefore, it transmits rather than scatters light (Fig. 4). Aerogel is an excellent thermal insulator because of its low density and extremely small pore size. A nonevacuated 1-inch-thick aerogel window would have an R value of about 7, which would climb to nearly R-20 upon removing 90% of the air. The goals of the project are to improve the optical and thermal properties of aerogel, develop methods to protect it from the environment, and discover less expensive synthesis methods to accelerate its introduction into the commercial window market.

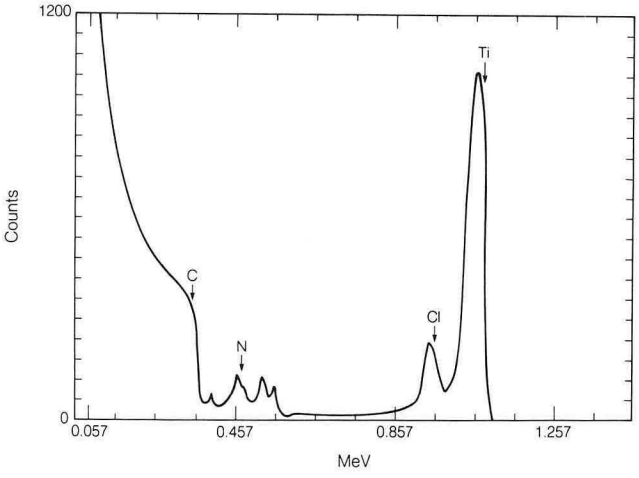

Figure 3. Rutherford backscattering spectrum for titanium oxynitride coating on glossy carbon substrate.
(XBL 854-9799)

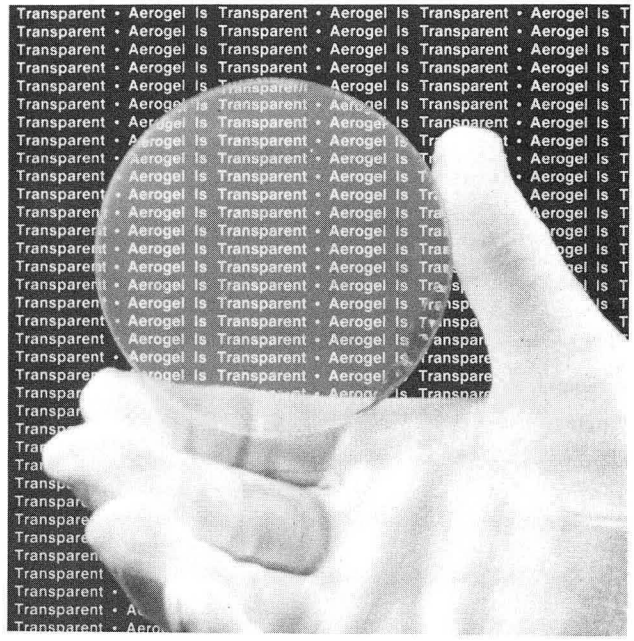

Figure 4. Photograph of a disc of aerogel, illustrating its transparency and image-preserving optical qualities.
(CBB 8410-7760)

Accomplishments During FY 1984

Preparation of Aerogel

Aerogel production has two stages: (1) preparation of an alcogel by hydrolysis and condensation of silicon-alkoxides and (2) drying of the alcogel to achieve the aerogel. The first step mixes alkoxide, water, and solvent to produce very fine particles in solution that link together to form an alcogel, a semisolid consisting of a silica matrix containing mainly alcohol. In the second step, the alcohol is removed to leave an open-pore silica matrix. We improved both these steps to make the process simpler and more economical.

We prepared aerogels from two silicon-alkoxide starting compounds: $Si\text{-}(OCH_3)_4$ (tetramethyl orthosilicate—TMOS) and $Si\text{-}(OC_2H_5)_4$ (tetraethyl orthosilicate—TEOS). Good-quality transparent aerogels were made from base-catalyzed TMOS. Although TMOS is quite toxic, the final aerogel product is completely safe. To produce aerogels on a commercial scale, however, it would be desirable to use the much less toxic TEOS. Only acid-catalyzed TEOS had been used successfully to produce aerogel, and this displayed greater shrinkage and light scattering than did TMOS. A base-catalyzed process using TEOS was needed, and this we succeeded in developing. We then carried out experiments to optimize the process, using the factorial design tech-

nique. Concentrations of alkoxide, water, alcohol, catalyst, and process temperature were changed simultaneously. Properties including light-scattering, optical spectra, pH, rheology of the sols, shrinkage, and surface area were measured to optimize the process. These studies have helped us better understand the process chemistry and evaluate the significant parameters in preparing TEOS aerogels having the desired qualities.

Supercritical Drying of Alcogel

More than 90% of the alcogel volume consists of fine pores containing alcohol. This alcohol must be removed to produce aerogel. Air drying causes the alcogel to collapse because of the extremely high interfacial forces at the gas/liquid interface. To prevent this damage, the alcohol is removed from the pores under supercritical conditions that minimize the interfacial forces. For alcohols, supercritical conditions are 270°C and ~1700 psi pressure. Such high temperature and pressure makes the process expensive and time-consuming (2 to 3 days for each batch). In a major breakthrough, we simplified the drying process by substituting liquid CO_2 for alcohol and supercritically drying at 40°C and $\leqslant$ 1200 psi. The drying time for each batch was reduced to 8 to 10 hours, and the equipment is simpler and less expensive than for high-temperature, high-pressure supercritical drying. This new drying method is a significant step in bringing the process closer to commercial viability.

Thermal Analysis of Aerogel

The thermal conductivity of aerogel is important both for determining the insulating value of an aerogel window and for helping us understand and improve its thermal performance. This year we tested various methods for measuring these properties. The laser pulse technique enables us to rapidly measure small samples in a small evacuated chamber. Its accuracy, however, is questionable. Supplemental measurements by conventional hot-plate techniques are also inconclusive because of the difficulty in preparing large, flat samples. Preliminary results were sufficient for us to develop suitable analytical models to apply to future results.

Planned Activities for FY 1985

Experiments to optimize the preparation of TEOS will continue. Alternative methods of preparation will be explored. The initial experiments in supercritical drying will be extended by performing detailed measurements to compare the properties resulting from the two drying methods. Methods of comparison will include spectroscopy, light scattering, and electron microscopy.

We will prepare new aerogel samples of optimum dimensions and with appropriate coatings for thermal conductivity tests. We will determine the magnitude of radiative heat transfer independently to evaluate the potential for using absorbing additives to reduce the conductivity of aerogel. The properties of evacuated and gas-filled aerogel windows will be determined and compared to other window designs.

OPTICAL SWITCHING PROCESSES AND MATERIALS

Optical switching materials or devices can be used for energy-efficient windows and other passive solar applications. An optical shutter provides a large change in optical properties under the influence of light, heat, an electric field, or their combination. The change can occur as a transformation from a material that is highly solar transmitting to one that reflects over part or all of the solar spectrum (Fig. 5). A less desirable alternative would be a material that switches from highly transmitting to highly absorbing since some of the absorbed energy would enter the building. An optical shutter coating would control the flow of visible light and/or solar heat gain through a building window, thus performing an energy management function. Depending upon design, such a coating could control glare, modulate daylight admittance, and limit solar heat gain to reduce cooling loads, prevent overheating, and improve thermal comfort. Initial results from energy simulation studies of office buildings suggest that the dynamic control attainable with optical shutter coatings provides substantial economic benefits by minimizing cooling and lighting energy use, reducing peak electricity demand, and potentially reducing the chiller and heating, ventilating, and air-conditioning (HVAC) system size.

We consider materials that possess variable or reversible optical properties as potential candidates for an optical shutter. There are three classes of phenomena that may prove useful:

(1) Chromogenic materials, including electrochromic, photochromic, and thermochromic types.
(2) Physio-optic media, including mesogenic molecules or liquid crystals, and magneto-optic, electro-optic, and mechano-optic or deformable media.
(3) Electrodeposition, including reversible electrodeposition and electrophoresis.

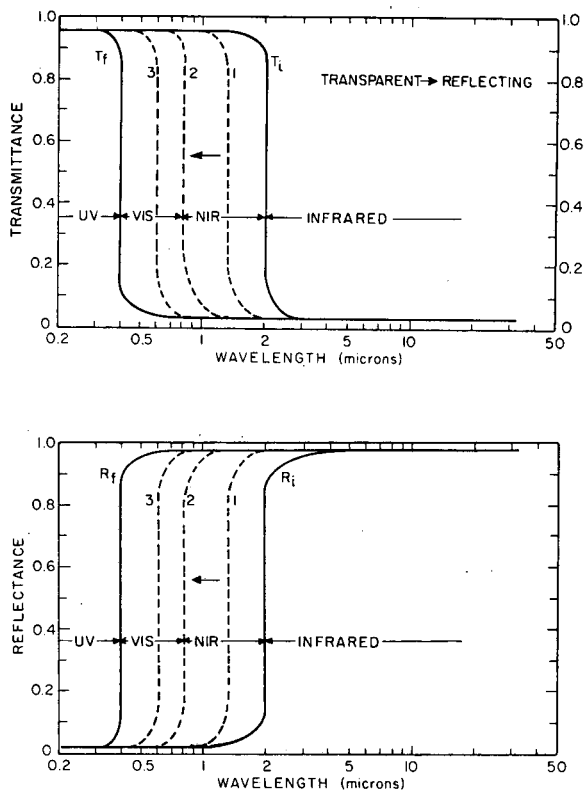

Figure 5. Idealized broadband spectral response for a solar optical shutter. This example ignores the effect of absorption and shows a highly transparent film transforming into a highly reflecting one. Such a shutter can control certain portions of the solar spectrum to provide or restrict both solar heating and lighting. (XBL 828-6452)

Our research program focuses on electrochromic coatings because they offer the potential for active control (by an applied voltage) in response to building operating requirements and environmental conditions and because there is sufficient experience with optical displays and related applications to suggest that they would be the best candidates for glazing applications. The active control capability will allow the greatest range of potential benefits in terms of reducing cooling loads, providing daylighting savings, controlling peak electricity demand, and reducing HVAC size.

ELECTROCHROMIC DEVICES

Electrochromism is exhibited by many inorganic and organic materials.[4] An electrochromic material undergoes an intense color change when a colored compound is formed from an ion-insertion reaction induced by an instantaneous applied electric field. The reaction might follow:

$$MO_x + yA^+ + ye \rightleftarrows A_yMO_x \quad .$$

There are three categories of electrochromic materials: transition metal oxides, organic compounds, and intercalated materials. The materials that have attracted the most research interest are WO_3, MoO_3, and NiO_x films. With organic electrochromics, coloration of a liquid is achieved by an oxidation-reduction reaction, which may be coupled with a chemical reaction. Intercalated electrochromics are based on graphite and so are not useful for window applications.

A solid-state electrochromic device containing the elements shown in Fig. 6 can be fabricated: a transparent conductor, an electrochromic layer, an electrolyte or fast-ion conductor, a counter electrode, and a second transparent conductor. Many variations on this configuration are possible, although several of the approaches used for small electronic displays cannot be scaled up successfully to the dimensions required for windows.

Accomplishments During FY 1984

Prior to 1984, a technical review of electrochromism revealed many possible materials that could be incorporated into solar glazings.[4] During 1984 our research focused on electrochromism in nickel oxide, which can be switched from transparent to bronze or dark gray, depending on impurities. We performed experiments on oxidized metal films and chemically deposited oxides on indium-tin-oxide coated glass. We obtained a normally transmitting film with solar transmittance (T_s) and visible transmittance (T_v) as follows: T_s (off) = 0.73, T_s (on) = 0.37, and T_v (off) = 0.75, T_v (on) = 0.24. The spectral response is shown in Fig. 7. In an electro-

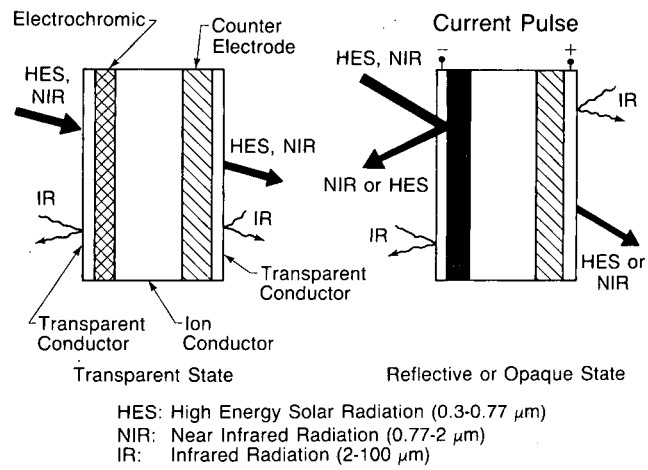

Figure 6. Schematic of an electrochromic optical switch shown in each of two states, transparent and colored. A current pulse causes an ion-based chemical reaction to take place in the electrochromic material. (XBL 842-10105)

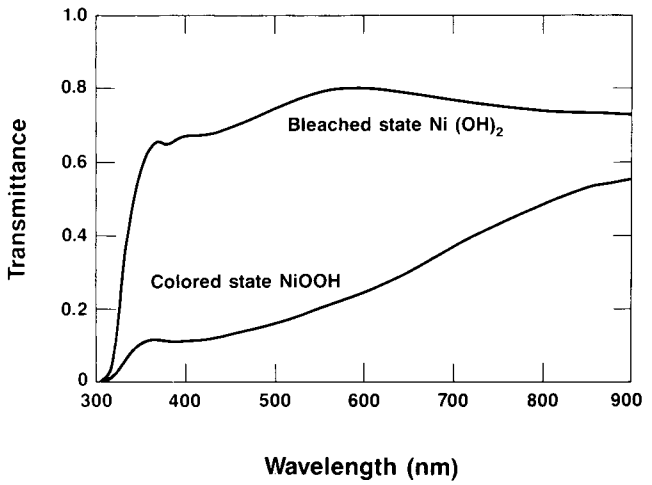

Figure 7. Transmission (near-normal) spectrum for nickel hydroxide in bleached and colored state. Conditions are IM-KOH electrolyte with 1 V applied potential. (XBL 852-6955)

chemical cell, 1 volt is required to switch the film. Besides spectrophotometry, voltammetry and Auger electron spectroscopy were performed on this film. These studies will help determine the active species in the electrochromic coloration reaction.

LBL continues to serve as scientific coordinator for the overall DOE-supported switching films program. Associated research was continued in 1984 by EIC Laboratories[5] and the Department of Electrical Engineering at Tufts University.[6] Electrochromic near-infrared reflectance modulation was demonstrated in polycrystalline WO_3 material.[7] Devices based on the configuration in Fig. 6 and with complementary electrochromic electrodes were made. Research by the Solar Energy Research Institute (SERI) has concentrated on devices based on amorphous WO_3 in the configuration: transparent conductor/WO_3/ion conductor/Au or indium-tin-oxide.[8]

Planned Activities for FY 1985

We will complete optical, chemical, and structural studies of electrochromic nickel oxide. We will compare the electrochromic response of sputter-prepared nickel oxide materials to the electrochemically prepared coatings. With our new reactive magnetron sputtering system, we will begin to survey and characterize electrochromism in other candidate materials such as titanium oxide. The objective of this work is to identify and characterize electrochromic materials with performance characteristics that are better than the commonly used WO_3 films.

OTHER SWITCHING FILM MECHANISMS

A number of other materials systems were reviewed to determine their suitability as optical switching materials. We continue to follow development of photochromic and thermochromic materials to determine if any may prove suitable to building applications. We also examined various physio-optic processes (i.e., liquid crystals, magneto-optic and electro-optic materials) as well as processes based on reversible electrodeposition and electrophoresis. Each approach has at least one attractive feature, but in general they appear less promising than the alternatives described above.

Accomplishments During FY 1984

An example of a device studied in FY 1984 is the dynamically light-scattering liquid crystal cell. It transforms from transparent to opaque white under applied potential; no polarizers are required. Its optical properties are T_s (off) = 0.82, T_s (on) = 0.77, T_v (off) = 0.83, T_v (on) = 0.20. Although the response of this device (Fig. 8) is promising as a broadband optical shutter, it suffers from excessive power requirements and lack of uniformity over large areas.

Planned Activities for FY 1985

We will continue to follow these novel approaches for optical switching mechanisms to determine if results in other fields have relevance to aperture requirements. We expect to obtain samples of photochromic plastics to determine their suitability for building applications.

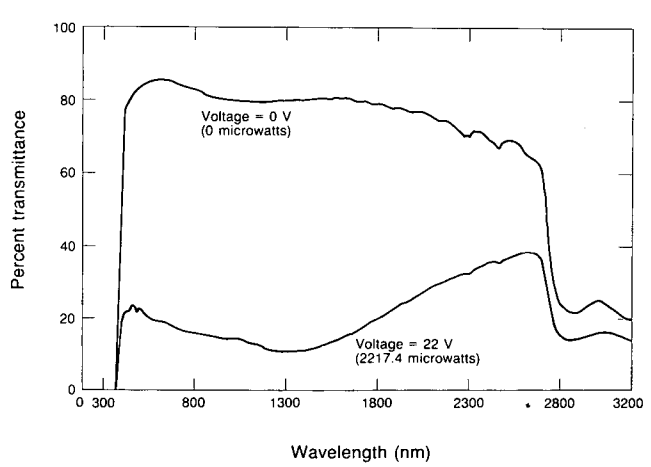

Figure 8. Spectral transmittance (near normal) for a dynamically scattering liquid crystal device. Response includes two glass cover plates and two transparent conductor electrode films. (XBL 852-7033)

MATERIALS FOR IMPROVED USE OF DAYLIGHT

The intensity and spatial distribution of daylight transmitted through windows and skylights must be controlled in order to reduce electric lighting requirements while maintaining occupant comfort. Conventional solutions rely on architectural elements and interior or exterior devices to control daylight admission and distribution. Greatly improved performance would result from materials or systems that could: (1) transmit maximum daylight with minimal cooling load impact (i.e., reject solar infrared radiation); (2) collect and distribute daylight beyond the perimeter zones in buildings; and (3) provide angular selectivity in accepting and redirecting incident light at the building envelope.

In earlier studies, we evaluated the performance of a variety of devices for daylight acceptance and control on the basis of their reflective and refractive optics. In 1982, we turned our attention to innovative optical materials and devices that showed the potential for replacing more complex mechanical systems. We reviewed the feasibility of approaches such as fiber-optics systems, hollow light guides, holographic coatings, selective-reflectance materials, and various scattering media. One promising approach that uses fluorescent concentrators to collect and redirect daylight is the subject of a patent disclosure.

LIGHT GUIDES

Accomplishments During FY 1984

In 1984, on the basis of the preceding year's review of potential systems for light guides, we focused on two promising areas. We predicted improved performance for hollow reflecting light pipes because of the availability of new low-cost materials of high reflectivity (more than 95%). Figure 9 shows the calculated transmission efficiency of this type of light guide as a function of aspect ratio (length/diameter) for R = 95%. Even for aspect ratios of 50 (e.g., L = 15 m, D = 0.3 m) the transmission has acceptable values at moderate concentration angles. We also investigated the performance of plastic optical fibers and evaluated the potential for improvement through further purification of the base polymer.

Planned Activities for FY 1985

We will continue our investigation of hollow reflecting light guides. Available reflecting materials will be completely characterized and the results used in improved analytical models. We will compare these model results with the actual performance of hollow prismatic light guides. Scale models of light guide elements will be tested in our sky simulator.

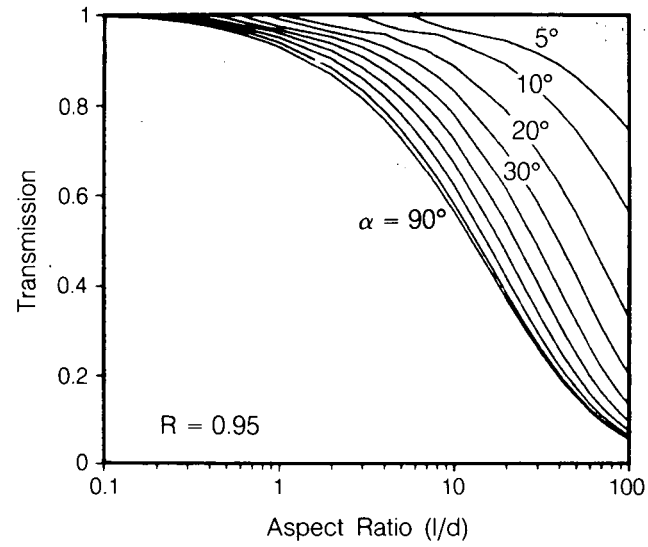

Figure 9. Transmission efficiency of a tubular light guide vs. aspect ratio (length/diameter); α is the half-angle of the concentrated sunlight and R is the inner surface reflectivity. (XBL 854-9798)

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Active Solar Cooling*

M. Wahlig, K. Dao, M. Warren, J. Rasson, R. Armer, P. Brothers, A. Heitz, A. Shavit, D. de Silveira, and T.-C. Tsao

This project has three major tasks: (1) research on improved absorption cycles for high-efficiency active solar cooling and heating systems; (2) systems and economics analysis of active solar cooling and heating systems to establish operating requirements, research needs, and thermal performance of current and advanced space conditioning systems; and (3) technical support activities for the Department of Energy's active solar cooling program.

Absorption Chiller Research

The objective of the research on absorption-cycle chillers is to achieve a significantly higher conversion efficiency than is possible in other approaches to solar cooling and heating of buildings. Being essentially heat pumps, absorption-cycle chillers can be used for heating as well as cooling if the refrigerant fluid does not freeze in the outdoor coil during heating applications. We restrict our fluid choices to those for which this heating option is available.

The absorption-cycle research program consists of four phases, each successive phase leading closer to the final machine. The first phase was successfully completed some time ago.[1] By modifying a conventional gas-fired ammonia/water absorption chiller, we demonstrated the capability of our analysis techniques to predict accurately the performance of single-effect (i.e., single-stage) absorption-cycle chillers under operating conditions appropriate for solar-powered cooling.

In the second phase, a completely new solar-driven single-effect chiller was designed, fabricated, and tested, using the experience gained during the first phase. This ammonia/water chiller had several unique features for recouping thermal and mechanical energy. The second phase was successfully completed[2] in FY 1982.

In the present, third phase, we are investigating the performance improvement obtained by adding a unique second stage to the single-effect chiller tested in the second phase. The resulting double-effect regenerative cycle (or cycle 2R) has been described previously.[3] Basically, with the addition of the second stage, the overall chiller efficiency increases continuously as a function of the inlet temperature from the solar collectors. This 2R chiller has been designed,[4] fabricated, and assembled; the debugging and testing was started in FY 1983 and will conclude in FY 1985.

In the fourth phase, a new concept in refrigeration-absorption cycles—one that should yield a still higher efficiency while requiring less heat-exchanger area, for a potentially lower cost—will be investigated. The basic concept of this single-effect regenerative cycle (which we call cycle 1R) has also been described previously.[5] A version of the 1R cycle will be designed in FY 1985. The success of the cycle 1R chiller depends on our experience in developing the cycle 2R chiller. A refrigerant-absorbent fluid pair with suitable properties at 300°F or higher, if it can be found, should further increase the efficiency of the 1R chiller.

Systems and Economics Analysis

The objectives of the systems and economics analysis activities are: (1) to perform system simulation and analysis of active solar absorption and Rankine cooling/heating systems to establish the operating requirements and thermal performance of current and advanced space conditioning systems; (2) to use the results of these analyses to determine future research needs for the solar cooling program, discovering where improvements can and must be made in thermal and electrical performance; (3) to evaluate by computer simulation the impact of system controls and control strategies on annual energy savings for active solar cooling and heating systems; and (4) to coordinate active solar cooling system simulation efforts under way by various groups (e.g., the Solar Energy Research Institute [SERI], Colorado State University [CSU], the University of Wisconsin) and maintain an archive of solar cooling system and component models developed in previous simulation work.

Technical Support Activities

Our technical support activities provide assistance for the active solar cooling program to the DOE San Francisco Operations Office (DOE/SAN) Fossil, Geothermal, and Solar Division and to the DOE Headquarters (DOE/HQ) Office of Solar Heat Technologies, Active Heating and Cooling Division. These activities include program planning; technical monitoring and evaluation of ongoing projects, including site visits and review of progress reports;

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coordination of review of unsolicited proposals; assistance in the preparation and evaluation of responses to program solicitations; and coordination of related activities by other organizations.

ACCOMPLISHMENTS DURING FY 1984

Absorption Chiller Research

Tests of the 2R chiller were performed and modifications made throughout FY 1984 and into FY 1985. Stable and efficient operation of the chiller has been achieved. Most of the problems related to fluid flow and liquid/vapor separation that had previously limited chiller performance were successfully resolved by the end of FY 1984. Only two major problems remain to be fully overcome, namely:

- Poor heat transfer characteristics of absorbers.
- Mechanical failures of the multistage pump.

Results of typical experimental runs made near the end of FY 1984 are summarized in Table 1.

Systems and Economics Analysis

Principal accomplishments during FY 1984 include:

(1) Evaluation of different storage control strategies for active solar cooling;
(2) Development of a TRNSYS simulation that includes chiller, cooling coil, and building-zone control characteristics to study the effect of resetting the chilled water temperature on solar absorption chiller performance;
(3) Preparation of a development plan for a new advanced absorption cycle simulation tool; and
(4) Completion of two review chapters for the DOE Documentation Project on active solar cooling and heating system costs and performance.

Two-Tank Storage Strategies

Controls play an important role in the effective operation of solar space-conditioning systems.[6] Storage-related control strategies have been analyzed with emphasis on methods of controlling the operation of two-tank storage systems so as to optimize cooling and heating system performance.

We have developed a storage model for TRNSYS that includes a second, small buffer storage tank. Control strategies evaluated for the two-tank system include a "switched" configuration (Fig. 1) and a "bypass" configuration (Fig. 2). Because chiller systems operate much of the time at less than 50% of design load, it is important to examine the performance effectiveness of different system configurations and control strategies with hourly simulations. These storage strategies have been compared with results for a system with a single stratified storage tank having the same volume.

Preliminary results of simulations for Phoenix and Miami in the month of June indicate a significant performance improvement for the "switched" storage configuration. Depending on system sizing and location, there is an improvement in the solar

Table 1. Results of typical 2R chiller experimental runs.

Capacity (tons)	Boiler temperature (°F)	Condenser temperature (°F)	Absorber temperature (°F)	Evaporator temperature (°F)	Experimental COP[a]
2.4	227	100	95	40	0.91
2.3	199	102	97	53	0.94
3.0	244	103	95	51	1.15
2.5	197	88	82	38	1.01
3.5	243	90	80	36	1.20
3.2	194	88	79	50	1.33
3.3	226	91	82	50	1.43
3.0	263	86	76	32	1.26

[a]Coefficient of performance.

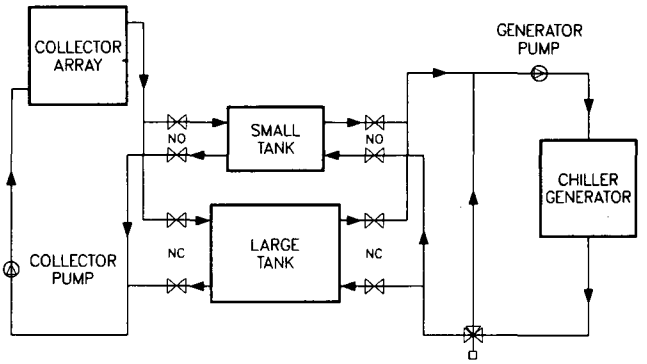

Figure 1. Two-tank "switched" storage configuration. (XCG 849-13266)

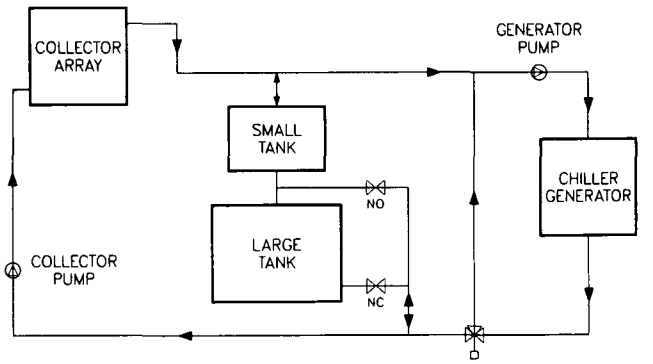

Figure 2. Two-tank "bypass" storage configuration. (XCG 849-13264)

fraction of from 5% to 15% and an improvement in the solar utilization (solar cooling performance factor) of from 3% to 15%. This system collects less energy over a month than stratified storage but produces more cooling because the collected energy is at higher temperatures. The "bypass" storage system also performs better than the stratified system, but not as well as the switched configuration.

Chiller Control Modeling

The performance of conventional chillers can be improved by resetting the chilled-water temperature upwards from 45°F to 55°F, provided that there is adequate dehumidification and an adequate supply of air to meet the demand. Because solar-driven chillers operate under varying conditions, such a temperature-reset strategy may improve their performance even more than in the case of conventional chillers. Two chiller control strategies that are expected to improve performance are: (1) reset of the chilled-water output temperature (upwards from 45°F to 55°F or even higher) when a higher temperature is sufficient to meet the sensible and latent loads of the building and (2) reduction of the chiller capacity when a lesser capacity is sufficient to satisfy the building load.

A TRNSYS simulation has been developed that models the thermal response of multiple zones, thermostat, variable air volume (VAV) system, fan coil, discharge-air temperature controller, economizer cycle, and conventional chiller.[7] The simulation keeps track of space humidity, air volume, and fan energy requirements in a simple building model. A conventional reciprocating chiller model has been adapted to include the effect of chilled-water and discharge-air temperature reset. The cooling coil model has been adapted for several options in the control of supply-air discharge temperature: (1) variable chilled water flow (mixing valve), (2) constant flow (pump) and diverting valve, and (3) constant flow and chilled water reset. Also, a detailed model of the discharge-air temperature coil has been implemented in the computer program TUTSIM[8] to understand the control and dynamics of a cooling coil in a VAV system.

Advanced Absorption Cycle Analysis

A new effort to develop a simulation model for evaluating the performance of advanced absorption-cycle machines was begun in FY 1984, building upon LBL's expertise and experience in simulation analysis and innovative absorption-chiller technology.

The goal is to develop a computer simulation model to predict the performance of advanced-cycle absorption machines in both cooling and heating modes. It is expected that the computer program will use modular subcomponent routines, variable time-step integration, and graphic presentation of results. The simulation program will be capable of predicting steady-state performance and may, in refined versions, be able to predict dynamic performance.

A review of previous models of absorption chiller cycles was completed in FY 1984, and a draft development plan for a new simulation tool was written.[9] In addition, a simple thermodynamic state point program has been developed to test the concept.

Other Activities

Publications. In FY 1984, two chapters were prepared for the DOE Solar Program Documentation effort: "Cost Requirements—Active Solar Heating and Cooling"[10] and "Comparative Performance and Costs of Solar Cooling Systems."[11] Also, a technical paper entitled "Cost and Performance Goals for

Commercial Active Solar Absorption Cooling Systems,"[12] has been accepted for publication.

Technical Coordination. LBL continues to play an active role in coordinating systems analysis activities for the active solar cooling program. In FY 1982, we worked actively with Science Applications, Inc. in identifying systems that needed to be simulated. In FY 1984, we worked with SERI in identifying simulation requirements and served as technical coordinator of the Drexel University solar controls evaluation project. This entailed working with Drexel and CSU to define the technical approach, instrumentation, and data acquisition requirements and coordinating with SERI, DOE/SAN, and DOE/HQ.

Technical Support Activities

Technical monitoring of solar cooling research projects being performed by outside (non-LBL) contractors continued through the first half of FY 1984. Seven site visits to four contractors were conducted. In addition, LBL coordinated the review of 16 topical and final reports written by the outside contractors.

LBL maintained cognizance of the progress of each outside research project though review of monthly progress reports and by frequent phone and mail contacts. LBL prepared and sent to DOE/SAN monthly summary reports on all the DOE solar absorption and Rankine cooling projects.

During FY 1984, LBL assisted DOE/SAN in preparing the technical sections of three "Requests for Proposals" concerning (1) comparative analysis of solar heating and cooling alternatives, (2) open-cycle solar cooling, and (3) advanced solar heating and cooling concepts. LBL staff also participated in the technical review of proposals received in response to these solicitations.

LBL staff participated in the following workshops and meetings: (1) DOE/Solar Workshop on the National Solar Data Network in November 1983, (2) DOE/Conservation Workshop on Building Energy Equipment in December 1983, (3) review meeting on the U.S.–Saudi Arabia SOLERAS Program organized by Midwest Research Institute in August 1984, and (4) topical review meeting on desiccant cooling conducted by SERI in September 1984.

LBL also provided technical inputs to DOE/SAN and DOE/HQ for annual and multiyear active-solar program planning documents. In related activities, LBL participated in systems analysis planning meetings coordinated by SERI and in overview meetings for the active solar program "research requirements" planning process.

LBL assisted DOE in drafting a proposed project on solar adsorption cooling and heating—Annex VIII of the U.S.–Israel Agreement in Energy Research and Development. This project is scheduled to start in FY 1985, with the technical tasks being performed by the Technion-Israel Institute of Technology in Haifa, Israel, and by LBL.

Frequent discussions with SERI staff members working on the solar desiccant cooling program facilitated coordination of the overall DOE solar cooling program, comprising absorption, Rankine, and desiccant cooling elements. Numerous discussions with staff members of Oak Ridge National Laboratory (ORNL) similarly helped to coordinate the absorption heat pump research activities supported by DOE/Conservation (for which ORNL provides technical support) with the absorption cooling activities supported by DOE/Solar. Frequent meetings during the first half of the fiscal year at DOE/SAN facilitated the necessary coordination between LBL's technical support effort and DOE/SAN's program management responsibilities for the solar cooling program.

In mid-FY 1984, redirection by DOE reduced technical support activities by about an order of magnitude (i.e., 90%) for the balance of the fiscal year. These activities are not expected to continue in FY 1985.

PLANNED ACTIVITIES FOR FY 1985

Absorption Chiller Research

Testing of the 2R chiller in the cooling mode will be completed early in FY 1985. An experimental performance map for the chiller will be determined over a representative range of operating temperatures and capacities. Most of the testing will be done using electrical diaphragm pumps as temporary substitutes for the internally vapor-driven multistage pump that is being developed. Work on the latter will continue, especially on its seals.

Absorber heat transfer enhancement will be investigated experimentally in FY 1985. This task will provide important input for the detailed engineering of the 1R chiller, currently scheduled for late in FY 1985.

Systems and Economics Analysis

Evaluation of Storage Options

Work started in FY 1984 will continue into FY

1985. Using improved chiller and cooling system models, we will evaluate the relative performance consequences of using sensible-heat or latent-heat storage subsystems on either the hot side or the cold side of the chiller.

A simplified approach has been developed to design and size the chiller and storage capacities, using an "available cooling" approach for an "average day," a "maximum day," and a "maximum storage day" for each month.[1–15] Simplified methods for design, sizing, and performance prediction based on this availability analysis will be applied to different storage options for active solar cooling systems. Results of these simplified methods will be compared with detailed TRNSYS simulations to establish cooling-system design guidelines. A major report on storage for active solar cooling systems will then be prepared. The report will contain the results of these simulations, an evaluation of the relative merits of the various storage strategies, and a description and evaluation of the simplified analysis methodology.

Advanced Solar Cooling System Analysis

In FY 1985, simplified methods and detailed TRNSYS simulations will be made to establish solar cooling system performance using advanced chillers. Both ideal chiller models (based on percentage of Carnot performance) and performance-map chiller models (based on the characteristics of advanced cycles) will be used. The results of the analysis using ideal chillers will set upper bounds for performance and economics of advanced absorption systems.

Approximate performance maps for several advanced-cycle absorption chillers have been generated (analytically) over the past year or so, and these are the prime candidates for inclusion in the performance analyses to be carried out here. Among these devices are the advanced-cycle absorption chillers and heat pumps of Carrier, Trane, Phillips, LBL, and the University of Texas. System performance analyses of two or more of these chillers will be conducted. The results of the detailed TRNSYS simulations for each chiller type will be compared with the predictions of the simplified methods.

As part of this task, the performance of advanced absorption systems will be compared with that of conventional and desiccant systems. The contributions due to indirect and direct evaporative cooling and to sensible heat exchange between the supply and exhaust air will be evaluated for the different systems.

Technical Support Activities

These activities are expected to conclude by the end of FY 1984.

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Photochemical Conversion of Solar Energy by Biological Systems*

L. Packer, R.J. Mehlhorn, A.T. Quintanilha, E. Robinson, E. Hrabeta, S. Wu-Chou, J. Herz, and E. Lam

The Membrane Bioenergetics Group is studying biological energy converters, emphasizing light-energized systems with relatively simple structures. These systems show promise for eventual technological applications as photoelectrical generators and electrical storage devices, either as isolated from the organisms or as chemically derivatized analogues of the biological catalysts. The principal research objective is to elucidate the molecular mechanisms of energy conversion by these photocatalysts. Bacteriorhodopsin (BR) has been the primary focus of this research program; last year the project was expanded to include bacterial chromatophores, which lack the water-splitting photosystem II of higher plants.

Bacteriorhodopsin is a relatively low-molecular-weight protein found in the purple membranes of the halophilic (salt-loving) bacterium *Halobacterium halobium*. The function of this protein in the bacterium is known to be the active pumping of protons from the cytoplasm to the external aqueous phase, using light energy at wavelengths of about 570 nm. Unlike the pigments found in higher plants, bacteriorhodopsin acts as a direct photoelectrical device, without the participation of electron-transport proteins. This simplicity of action as well as its remarkable stability in isolated purple membranes has generated intense, worldwide interest in how BR achieves its energy conversion. Research in other laboratories has yielded the primary amino acid sequence, resolved electron density data to 7 angstroms, and brought information about the position of the light-absorbing moiety, retinal. Studies in our laboratory have been concerned primarily with identifying the specific amino acids that actively participate in BR function.

Our basic strategy for studying the roles of specific amino acids in bacteriorhodopsin consists of altering the structure of BR with chemical reagents of high specificity to learn how the various amino acids contribute to photon capture and the subsequent proton pumping.[1] We routinely assay, with spectrophotometric and laser flash photolysis techniques, BR absorption spectra and the kinetics of the photocycle, both in isolated purple membranes and in sealed envelope vesicles derived from the bacteria. We also perform proton-pumping assays with sealed membrane preparations, including lipid vesicles that have been reconstituted with modified purple membranes. Because there are multiple appearances of all the amino acids that occur in BR, it is difficult to label only a single one and to assign a functional significance to it. Most of our studies have thus analyzed the effects of multiple labeling under various modification conditions and have sought to characterize the spatial distribution of labeled sites within the protein by structural analyses. In previous years we elucidated the roles of lysines, arginines, tyrosines, tryptophans, and carboxyl residues in the activity of the protein. We have shown that some of these amino acids are in close proximity to the retinal chromophore, whereas others are involved directly or indirectly in conducting the proton across the membrane.

We have also experimented with retinal-deficient, mutant-derived "white membranes" that can be converted to spectroscopically normal purple

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membranes by adding retinal. These preparations of retinal provide novel research opportunities for us because they can be chemically modified when the normal retinal binding site is not occupied. White membranes also have quite different physical properties than purple membranes.

ACCOMPLISHMENTS DURING FY 1984

Table 1 summarizes what we have learned from chemical modification studies of bacteriorhodopsin. We have shown that perhaps three tyrosine residues participate in the proton-pumping activity of BR. In addition to the reversible protonation of tyrosyl groups, the participation of carboxyl residues is essential to the photocycle. However, lysine groups, long considered as potential candidates for the site of proton translocation, do not appear to be directly involved.

Table 1. Synopsis of information on bacteriorhodopsin from chemical modification and spin-probe studies.

- Three tyrosines are proton acceptors and/or donors: two at sites 26 and 64 (revealed by *iodination*), and one within the 72–248 proteolytic fragment (shown by *nitration*).
- Reprotonation requires the participation of ion pairing between carboxyl and arginine groups.
- At least one carboxyl group is deeply imbedded within the hydrophobic core of BR (from *spin labeling of carboxyls*).
- The O_{640} intermediate is related to the blue acid species.
- Photocycle kinetics is regulated by the proton-pumping force (from *electron spin resonance studies*).
- Intermolecular motion is not a prerequisite for function (from *crosslinking data*).
- Intramolecular conformational freedom is essential for function (from *crosslinking data*).
- The cytoplasmic tail is partially immobilized, and is required for full activity (*spin labeling of carboxyls, proton/M_{412} stoichiometry*).
- Tryptophans interact with retinal (*iodination*).
- Zero-length crosslinking alters the pattern of proteolytic cleavage.

Short-range molecular motion appears to be essential for activity because crosslinking inhibits the reprotonation phase of the photocycle, particularly zero-length crosslinking occurring between lysine and carboxyl residues. The latter observation has been exploited recently to show that selective patterns of proteolytic cleavage of bacteriorhodopsin can be accomplished following such intermolecular crosslinking.

Selected detailed results of our recent studies are presented below.

Tyrosine Modification

BR contains 11 tyrosines whose titratable hydroxyls are plausible candidates for conducting protons across the membrane. We have employed two strategies for modifying this amino acid: iodination of surface groups with the membrane-impermeable reagents glucose oxidase and lactoperoxidase and nitration with tetranitromethane.[2–5]

Iodination showed that the tyrosines most sensitive to alterations in their photocycle kinetics are located at or near the cytoplasmic surface of the purple membrane. Correlation of an altered pH-dependence of proton-pumping activity with pK_a shifts of iodinated tyrosines has implicated tyrosines as donors and/or acceptors in the proton conduction pathway.

Nitration caused blue shifts in the absorption spectrum, suggesting that tyrosines play a role in determining the absorption spectrum of BR. Nitration also induced changes in the circular dichroism spectra of purple membranes that could be ascribed to a weakening of the interaction between neighboring BR molecules. When nitration was performed under illumination at low pH, we discovered a new light-dependent nitration reaction having a considerable improvement in its specificity—a single tyrosine residue could be modified under the reaction conditions. Nitration in the dark at alkaline pH caused one type of blue shift, whereas nitration in the light at acidic pH affected another tyrosine and caused a different blue shift. This new modification, together with results from other laboratories, suggests that at least 3 of the 11 tyrosine residues are essential for proton-pumping activity.

Carboxyl Modification

We have applied a water-soluble and a hydrophobic carboxyl-activating reagent to BR to probe the occurrence of acidic amino acids in environ-

ments of different polarities.[6–8] A hydrophobic quinoline, N-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline (EEDQ), has been used to activate primarily carboxyls that are buried within the nonpolar interior of BR.

Polar carboxyl groups in BR were activated with the water-soluble reagent ethyldimethylpropylamine-carbodiimide (EDC). Activated carboxyls will react with available nucleophiles to form amide bonds. If lysine residues within BR are in sufficient proximity, they will react with the activated carboxyls, thus effecting intramolecular (and perhaps intermolecular) crosslinkages. This might be expected to reduce the capability of BR to undergo energy-linked conformational changes. Indeed, we have observed that crosslinked BR has altered photocycle kinetics and is substantially impaired in its ability to pump protons.

When crosslinking is partially prevented by treatment with an exogenous nucleophile, e.g., glycine methyl ester (GME), less inhibition is observed. (GME was chosen as a nucleophile in this reaction because the extent of the reaction is easily determined with an amino acid analyzer. Other useful nucleophiles are aminoethylsulfonic acid [AES], whose negative charge ensures that the ionic properties of BR will be conserved during the modification; nitrotyrosinemethylester, whose pH-sensitive chromophore yields data on energy transfer processes with retinal; and 4-amino-2,2,6,6-tetramethyl piperidine-N-oxyl [Tempamine], a spin-labeled reporter group.)

In the presence of an excess of GME, up to 12 of the 23 carboxyl-containing amino acids of the protein can be chemically modified. Interestingly, up to 10 carboxyls can be modified without any perceptible loss of structural integrity. Treatment of control and crosslinked preparations with proteolytic enzymes has enabled us to assign modified amino acids to specific BR fragments; this information in turn has helped to tentatively locate the carboxyls in the tertiary structure of BR.

Because of the abundance of labeled carboxyls in BR, it has been difficult to learn about the distribution of reacted carboxyls within the BR structure. This issue has been tackled with some success by using the technique of spin labeling.[9] With it, we have shown that at least one carboxyl group is located in the hydrophobic core of the protein, more than 16Å from the membrane interface. Moreover, the distribution of spin labels was unexpectedly heavily weighted toward nonaqueous amino acids. Apart from the important conclusion that ionizable groups can reside within hydrophobic domains of BR, the spin-labeling study has laid the groundwork for analyzing the labeling patterns from many chemical modification procedures. This will enable us to perform more incisive chemical modification studies of proteins in the future (see "Planned Activities").

Retinal Analogues

The retinal chromophore of bacteriorhodopsin can be removed under light in the presence of hydroxylamine, yielding the colorless bacterioopsin. This protein can be reconstituted as BR with retinal analogues to probe its interactions with the chromophore. In one collaborative effort[10] we have been preparing the way for mechanistic studies that will employ photoaffinity labeling with retinal analogues by using a derivatized "mesityl" retinal. Bacteriorhodopsin so reconstituted retains a photocycle, albeit greatly slowed, indicating that the substitution is in the same place as the native retinal.

QELS Studies

During the past 18 months we have collaborated with Bernard Arrio and Pierre Volfin (University of Paris, Orsay) in using laser Doppler velocimetry (LDV) and quasi-elastic light scattering (QELS) to evaluate accurately and quantitatively changes in the surface charge of purple membranes and purple membrane–containing vesicles (LDV technique) and the size distribution of purple membrane preparations (QELS technique). These studies have led to two important results.[11]

First, an absolute measurement of the surface charge of the purple membrane before and after chemical modification has been made, and light-induced changes in the surface charge have been determined in suspensions of purple membranes. In future studies, QELS may also help separate and characterize reconstituted liposomes containing purple membranes (with or without other catalysts) because it can directly visualize, and thus separate, populations of these vesicles moving at different velocities in an electric field.

Second, routine analysis revealed a striking difference in the mobilities of purple and white membrane preparations. Under applied electric fields purple membrane preparations migrated more slowly than white membrane preparations, implying that the effective sizes of the former were larger than the latter. Negative-staining microscopy in conjunction with QELS revealed that purple membrane preparations were aggregated or stacked, whereas white membranes were smaller and unstacked. We were able to show that this was, in effect, due to low-level proteolytic cleavage of the terminal tail. Subsequently we showed that controlled trypsin cleavage of the C-terminal tail produced a massive

aggregation of purple membrane preparations. Under these conditions membranes were observed, by electron microscopy, to be regularly stacked upon one another. This is readily explained by the removal of the highly charged C-terminal tail of 21 amino acid residues and their 5 carboxyl groups; removal reduces the electrostatic charge with respect to the hydrophobic forces between purple membrane sheets. When such aggregated preparations are mixed with lipids and treated in such a way as to form reconstituted liposomes, these aggregates are apparently teased apart.

These findings suggest that the low values of proton-to-M_{412} stoichiometry (or cations released per M_{412} stoichiometry; M_{412} is an intermediate of the photocycle), reported in the literature as being lower for isolated so-called "native purple membranes" than for reconstituted liposomes, are artifacts that result from this stacking/aggregation phenomenon. This effect needs to be considered in evaluating all earlier studies reporting stoichiometries of cation-to-photocycle activity of suspensions of purple membrane fragments. Our results are consistent with, and provide insights into, previous controversies in the literature about these stoichiometries from the laboratories of Ebrey, Khorana, and Ovchinikov.

Development and Results of Spin-Probe Methods

We have pioneered novel tools for accurately measuring energy transduction phenomena involving biological membranes, including internal aqueous volume, pH and electrical potential, and membrane surface potential.[9] These tools have been successfully applied to four systems: halobacterial membrane vesicles, isolated and reconstituted purple membranes, and bacterial chromatophores. Our technique consists of observing electron spin resonance (ESR) spectra of nitroxide-stable free radicals within membrane-enclosed domains and inferring the concentrations of the probes from these spectra. Among the probes we use for this purpose are weakly polar nitroxides, whose intracellular signals are representative of cell volumes; spin-labeled amines and weak acids, whose intracellular spectra are indicative of transmembrane pH gradients; and spin-labeled hydrophobic ions, which provide information about electrical potentials. Since all these parameters are measured under nearly identical conditions, the results of our analyses are considerably more accurate than commonly used indirect assays of electrochemical potentials, such as measurements of radiolabeled tracers in flow dialysis experiments or studies with fluorescent dyes based on self-quenching effects.

ESR Studies of Halobacterial Membrane Vesicles

ESR methods with isolated halobacterial membrane vesicles have proved to be extremely useful for characterizing the activities of bacteriorhodopsin. With the methods described above, accurate changes in internal pH and changes as a function of external pH have been calculated. Since the proton-pumping function in naturally oriented BR vesicles is such that protons are pumped from the inside of the vesicles to the external medium, the probe of choice for light-induced pH studies is a spin-labeled weak acid, Tempcarboxylate. In reconstituted membrane vesicles made from isolated purple membranes and lipids, where the flux of light-induced proton translocation is from the outside to the inside, and in halorhodopsin vesicles, where protons passively follow the actively pumped chloride ions, the probe of choice has proven to be Tempamine. ESR experiments with membrane vesicles in sodium chloride versus potassium chloride media have permitted us to investigate and quantitate the action of the sodium proton antiporter (two-ion exchange) driven by the proton translocation activity of bacteriorhodopsin.

Equilibrium Between the Photocycle and the Proton Electrochemical Potential

Reconstituted bacteriorhodopsin liposomes have proved to be ideal for demonstrating, for the first time, that the proton electrochemical potential that can be generated by bacteriorhodopsin in a sealed membrane system is in equilibrium with the photoreaction cycle.[12] By combining the ESR spin-probe method for measuring volume, pH, and membrane potentials with illumination studies of the formation and decay of the M_{412} intermediate, we have been able to show that the amount of the M intermediate formed during steady-state illumination is diminished by reagents that collapse the membrane potential but not the pH gradient. This indicates that the proton-pumping activity is slowed by the development of a transmembrane electrical potential. Parallel studies with laser flash photolysis have shown that the transmembrane potential slows down the decay of the M_{412} intermediate but not its rise. These studies are being extended to assess the consequences of this type of regulation not only in reconstituted liposomes but also in native membrane preparations and intact cells.

Chromatophore Studies

Our recent studies with chromatophores have been concerned with measuring the pH gradients that are formed upon illumination.[13] We used nitroxide spin probes to show that these pH gradients reach a magnitude slightly greater than two units when the membranes are bathed in media containing relatively high concentrations of potassium. When no chemical reduction of the probes occurs (e.g., in chromatophores), the spin-probe technique has two significant advantages over commonly used alternatives for measuring bioenergetic parameters: (1) volume and pH measurements are made under virtually identical conditions and (2) membrane binding artifacts can be eliminated.

In further studies, we used single-turnover light flashes to show that protons are progressively released from the membranes, thus ruling out a postulated "proton sink" within the membrane interface (Fig. 1). Such potential wells had been invoked to suggest that measurements of electrochemical potentials in bulk aqueous media might underestimate the true potentials that could be generated within microdomains of energy-transducing membranes. The extremely high sensitivity of the spin-label method made these measurements feasible and permitted the detection of gradients resulting from a single turnover of proton-pumping proteins, e.g., bacteriorhodopsin.

PLANNED ACTIVITIES FOR FY 1985

Future studies will develop some of the recent discoveries made in our laboratory that address interesting, unsolved problems on the structural/functional relationships of bacteriorhodopsin in the purple membrane. We envisage studies in four areas:

(1) *Characterizing the structure of isolated preparations of "native" purple membranes and white membrane fragments in suspension.* These membrane preparations are used by virtually all laboratories that work with bacteriorhodopsin. Using QELS combined with negative-staining electron microscopy, our studies have shown that purple membrane preparations aggregate or are stacked on top of one another, whereas the white membrane preparations do not exhibit this behavior. This has profound consequences for measurements of accurate stoichiometries of cations (including protons) released during photocycle activity. Accurate information on these stoichiometries is necessary to understand the mechanisms of activity.

The highly charged C-terminal tail of BR appears to play an important role in the aggregation of purple membranes. Therefore further studies on the specificity of cleavage of the C-terminal tail of bacteriorhodopsin will be pursued not only with trypsin but also with other proteolytic enzymes such as papain, before and after chemical modification (with and without spin nucleophiles), to study the degree to which the C-terminal tail is released.

(2) *Characterizing the three-dimensional structure of BR.* A major unsolved problem in bacteriorhodopsin research is to relate the known primary sequence of the molecule to its tertiary structure in the membrane. Electron and neutron diffraction experiments have strongly suggested the existence of seven alpha-helical rods spanning the membrane. However, the correlation of individual rods with defined segments of the primary sequence has not been made. No single experiment yet performed gives an unambiguous assignment of the position of any one segment relative to another. This problem is of paramount importance in solving the structural/functional relationships involved in the energy conversion and proton translocation process.

Our recent studies[8] reveal that crosslinking with carboxyl-activating reagents without the addition of an external nucleophile causes a very short crosslink to occur in bacteriorhodopsin. We have found that such chemical modification results in selectivity in the pattern of proteolytic cleavage of segments of bacteriorhodopsin. This is potentially a clue for determining which part of the molecule has been crosslinked, intra- or intermolecularly, during this process. Since the gel electrophoresis data indicate some selectivity in the generation of dimers following such treatment, we ought to resolve which por-

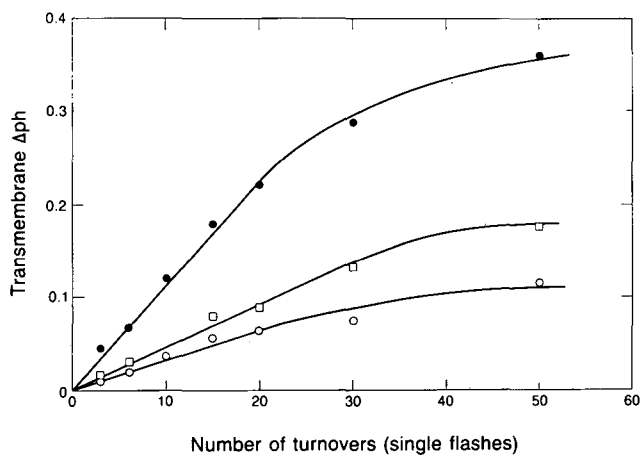

Figure 1. Measurement of pH gradients in chromatophores of *R. sphaeroides* with a spin-labeled amine (Tempamine) at concentrations of 1 m*M* (•), 2 m*M* (□), and 4 m*M* (o). (XBL 841-10031B)

tions of the bacteriorhodopsin molecules are adjacent and to identify their positions in the molecule. In collaborative studies we plan to examine these preparations with electron and neutron diffraction techniques. Chemical modification with deuterated reagents (in the case of neutron diffraction) may help to identify the positions of modified amino acids. Electron diffraction studies may reveal if there has been a change in the organization of the BR molecules in the plane of the membrane.

(3) *Membrane asymmetry and proton reactions.* Among problems of great interest in energy conversion are the asymmetry and localization of interacting cations with proton-pumping systems (localized versus delocalized protons). To study these problems it is essential to have oriented systems containing energy transduction. To further characterize these properties in bacteriorhodopsin we will employ liposomes containing modified bacteriorhodopsin. We will also continue some studies with bacterial chromatophores isolated from *Rhodopseudomonas spheroides.*

(4) *Development of improved chemical modification strategies for more selective reactions with amino acids.* Our main objective continues to be the unraveling of the mechanism of action of BR and other photocatalysts. We are convinced that more specific modifications of amino acids will enable us to obtain valuable new insights into the structural basis of bacteriorhodopsin activity. We will seek to improve the resolution of chemical modification by means of reagents that react only within specific membrane domains. This can be achieved by attaching the reagents to amphiphilic molecules whose strongly polar headgroups will bind specifically to the membrane interface and whose reactive residues are attached to the hydrophobic tails of the amphiphiles.

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LBL Building 71 Solar Cooling Project*

F. Salter

This active solar cooling project is part of the Department of Energy's Solar in Federal Buildings Program. The program is intended to demonstrate the federal government's confidence in the solar industry and to stimulate growth and technical improvements in solar technology through the installation and demonstration of a variety of commercially applicable solar energy systems in buildings owned or occupied by the federal government. The program provides technical and financial assistance through interagency agreements to federal agencies for design, acquisition, construction, and installation of solar heating and cooling equipment projects.

Building 71, which houses the Heavy Ion Linear Accelerator (HILAC), was chosen as the site for one of these demonstration projects. The LBL Plant Engineering Department is responsible for project engineering and contract administration. LBL's duties have included preparation of the project proposal, preliminary engineering, conceptual design, selection of design criteria, selection of an outside architect/engineer for final engineering and preparation of plans and specifications, engineering and administrative support for the architect/engineer, periodic review of the final design, and administration of the bid process and subcontract negotiations; present duties include construction supervision, acceptance testing, and field testing of the system. The LBL Active Solar Research Group provides technical assistance and review of the project.

Overall administration is provided by the San Francisco Operations Office of the Department of Energy (DOE/SAN). DOE/SAN has subcontracted technical management of the project to the Energy Technology Engineering Center (ETEC).

The Solar Cooling System will provide substitute capacity for the existing Building 71 chilled water system by installing a solar-driven chiller next to and in parallel with the existing electric chillers, which will be retained for back-up. The system will consist of roof-mounted collectors; storage tanks; a nominal 25-ton-capacity lithium bromide chiller package; and associated pumps, piping, insulation, valves and fittings, controls, and instrumentation. The chiller package was supplied by Arkla Industries, Inc., and will be field-tested in the system. The solar chiller is expected to operate at full load for an average of 6 hours per day.

Table 1 summarizes the design parameters of the cooling system. In addition, the collector array will use Energy Design HP-250 evacuated-tube solar collectors to accomplish the 250°F maximum design temperature. The collector design emphasizes simplicity and durability to minimize maintenance. This is essential, because roof radiation when HILAC is operating will restrict access to the collectors. Fluid will be contained in stainless-steel tubing so that glass-tube breakage will not disrupt system operation, and tube replacement can be scheduled for periods when the accelerator is not operating. Further reliability is accomplished by using high-quality Pyrex-type evacuated tubes that are less prone to breakage. Also, the collectors have no cover glass, making tube replacement easier.

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The solar collectors were installed in September and October of 1983, completing the installation of major equipment on the project.

Construction was partially stopped in December

Table 1. Parameters of LBL Building 71 solar cooling system.

Chiller capacity	25 tons (nominal)
Chiller COP	0.73
Average operation	6 hr/day (at 22-ton loading)
Generator entering-water temp.	185°F (adjustable 170°F to 200°F)
Exiting chilled-water temp.	45°F
Entering condenser-water temp.	80°F
Maximum storage temp.	250°F
Collector area	5100 ft^2 (gross area)
Collector type	evacuated-tube (198 collector modules, with 7 tubes per module)
Storage tank	2500 gallons
Thermal ballast tank	500 gallons
Expansion tank	500 gallons

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Solar Heat Technologies, Active Heating and Cooling Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

1983 because of lack of funds, but work resumed in August 1984.

A permanent deionization system was installed for the solar loop, and special cleaning, flushing, testing, and corrosion control operations were accomplished. This special work was necessitated by a manufacturing change from copper to stainless-steel collector tubing. (Both General Electric and Energy Design found that copper tubes and fins were subject to degradation from oxidation in evacuated-tube collectors. Energy Design's change to stainless steel has not been totally successful because of stress-corrosion cracking; this can occur in stainless steel at stagnation conditions in an evacuated-tube collector when significant chlorides and fluorides are present.)

After the above work was completed, the solar collectors were piped into the solar loop. By mid-September 1984 the solar system was essentially complete and ready for pressure and operational testing. Pressure tests revealed that 10 solar collector modules were leaking internally.

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Energy Design replaced the fluid circuits in the 10 leaking solar collectors, and the solar loop was placed in operation at the end of October 1984. The solar chiller was started up and made operational in December 1984. Removal of the solar collector covers during start-up and generation of hot water in the solar collectors revealed 28 broken or defective evacuated tubes and two additional collector modules with internal leaks. These solar collectors were repaired in January 1985. Final acceptance tests should start in February 1985.

This project has been selected by DOE for special instrumentation for the National Solar Data Network. Appropriate instrumentation will be installed after system acceptance.

Solar Energy Conversion Using Microstructured Materials: Direct Radiant Heating of Small-Particle Suspensions*

A.J. Hunt, J. Ayer, P. Hull, R. McLaughlin, F. Miller, R. Russo, and W. Yuen

The Solar Advanced Micromaterials Research and Development Group is investigating the use of microstructured materials for the collection, conversion, and control of sunlight. Research is in four main areas: (1) direct radiant heating of small-particle suspensions to produce useful fuels and chemicals, (2) radiant heating of small-particle suspensions to initiate reversible chemical reactions for thermal energy storage, (3) solar detoxification of hazardous chemical wastes, and (4) development of microporous optical materials. The development of transparent microporous materials for insulating windows (aerogels) is reported in the article "Optical Materials Studies" in this chapter of the Annual Report and in the article "Windows and Daylighting" in the Energy Efficient Buildings Chapter; the thermal storage work is reported in the Chemical Process Research and Development chapter. This article describes research in the use of particle suspensions as solar absorbers to produce useful fuels and chemicals and to detoxify hazardous chemical wastes. The work was initiated in FY 1983 with support from the LBL Director's Discretionary Fund and currently receives DOE funding.

For the past 6 years, we have been actively involved in developing solar thermal systems that are based on the direct absorption of concentrated sunlight by particles suspended in a gas.[1-4] The particles absorb sunlight and heat the gas to high temperatures for electric power generation or industrial process heat. The concept was established experimentally by the design,[5,6] construction, and successful solar test[7] of the ability of the Mark I 30-kW Small Particle Heat Exchange Receiver (SPHER) to produce high-temperature gas. Solar tests were conducted at the Advanced Component Test Facility (ACTF) at the Georgia Institute of Technology in FY 1982. The tests confirmed that (1) particle suspensions are effective solar absorbers, (2) high gas temperatures can be attained, and (3) the high-temperature region may be isolated from the surrounding walls. This last result formed the basis for extending the research to higher temperatures for

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thermochemical applications.

Another result of this successful test of the Mark I receiver is interest in continuing the development of high-temperature-gas receivers based on the SPHER concept for electric power production. The SPHER concept ranked high in a DOE-initiated comparative study of various high-temperature-gas receivers for small solar central-receiver thermal power plants.[8] It is anticipated that a conceptual power plant design study for a SPHER will be performed.

Direct high-temperature chemical processing using concentrated sunlight offers distinct economic advantages over thermal/electric power generated by other methods of solar conversion. This is especially true for chemical production processes that require electricity to reach very high temperatures. The direct use of sunlight to drive these reactions eliminates the considerable Carnot-cycle losses inevitable in the heat-to-mechanical energy conversion required to operate an electric generator. Current goals of the present DOE-funded project are to continue research and establish a technological base for the use of direct radiant heating of particle suspensions to produce fuels and chemicals. In particular, we are obtaining fundamental data regarding the optical, thermodynamic, and chemical processes involved in direct solar heating of gas-particle suspensions through a balanced program of analytical and laboratory studies.

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Our research focused on critical issues in radiantly driven chemical reactors and receivers[9] using small particles as the solar absorber. The thrust is to investigate the fundamental processes by which small particles absorb sunlight and transfer the resulting heat to the surrounding gas; this basic information may then be applied to the initiation of chemical reactions. A survey of the literature was conducted to discover reactions particularly suited to activation in a direct-radiant small-particle reactor such as the Solar Thermally Activated Radiant Reactor (STARR). A substantial number of reactions were identified as having the following desirable characteristics: (1) endothermic (thus able to store the sun's energy as a fuel or chemical product), (2) potentially able to use small particles as the absorber material and in some cases as a catalytic site for the reaction, and (3) having some prospect of taking advantage of the high flux and high temperatures available in a receiver using concentrated sunlight.

Analytical Studies

Radiant energy transfer through a particle-gas mixture is calculated by using Mie scattering theory coupled with an expression sometimes referred to as Beer's law. Computer codes were written to calculate the fraction of monochromatic radiant energy remaining after traveling a given distance through the particle-gas mixture for the single-particle scattering case. Inputs to this program are experimental values of the particle mass loading, particle size distribution, and values from the literature for the particle's complex index of refraction as a function of the wavelength. Another computer program was written to allow the incident radiation to have a spectral distribution like that of an arc lamp or the sun.

A new approach to calculating heat transfer rates from particles to gas was formulated. It is used to study the effect of particle size, flux density, and gas conditions on the equilibrium temperatures reached by radiantly heated particles. An expression was developed for the heat transfer at intermediate Knudsen numbers (the ratio of molecular mean free path to particle diameter), using the concept of an imaginary surface at an intermediate temperature between the particle and the bulk of the surrounding gas. This one expression predicts the correct result for both small particles (free molecular heat transfer) and large particles (continuum heat transfer) and provides for the first time an analytical formula at intermediate Knudsen numbers.[10] It is also in good agreement with earlier experimental studies as illustrated in Fig. 1.[11,12] This expression will be used to calculate particle and gas temperature differences within a radiant reactor.

Experimental Studies

A small-scale (2.2 kW) arc-image furnace was constructed in FY 1983 to simulate concentrated solar radiation in the laboratory. A high intensity xenon arc lamp was mounted at one focus of an ellipsoidal reflector, which reflects the light coming from the arc to the second focus of the ellipsoid. A two-dimensional translation stage was added in FY 1984. This stage provides stable mounting for the ellipsoidal reflector, ensuring reproducible flux profiles. A similar, but three-dimensional translation stage was also made to allow precise positioning of the reactor vessel at the focus of the reflector and to serve as a scanning mount for a calorimeter when making spatial measurements of the radiant flux.

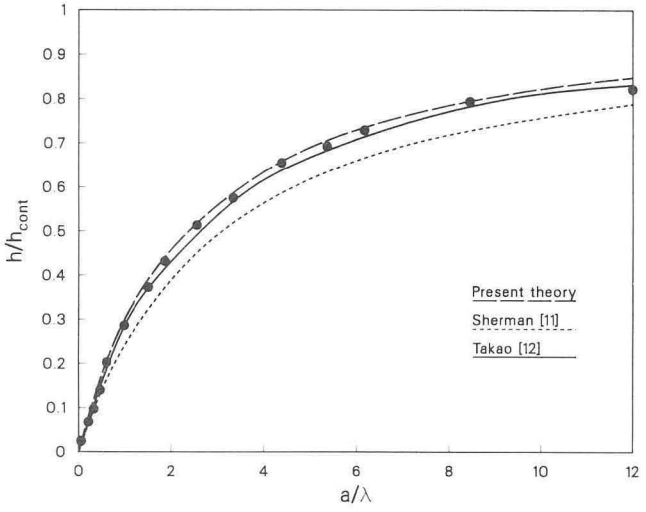

Figure 1. Graphs of a dimensionless heat transfer coefficient, h/h_{cont}, as a function of the ratio a/λ, where h is the heat transfer coefficient from a sphere to a rarefied gas, h_{cont} is the heat transfer coefficient from a sphere to a continuum, a is the radius of the sphere, and λ is the mean free path of the gas molecule. The points represent experimental data presented in Ref. 12. (XCG 851-41)

These measurements were made in the vicinity of the second focus of the reflector, and the total power entering the reactor was determined by a spatial integration. The measurements indicate a peak flux density on the order of 4000 kW/m^2, and a total power of 490 watts can be achieved within the reactor vessel, assuming an 8% reflection loss at the vessel window.

From these measurements, we also created a detailed three-dimensional map of the flux density that was used in the design of the first-generation quartz receiver/reactor. The gas-particle mixture enters the reactor vessel at the top and is exhausted near the bottom through a central tube. Light from the solar simulator passes through the quartz bottom of the reactor vessel and is focused just below the exhaust tube, ensuring that all particles pass through the highest intensity portion of the beam. This first reactor had a cone-shaped bottom to allow larger particles to fall into the apex and thus not block the main light beam. However, large particles were not found there after heating, so a second reactor with a flat bottom was constructed, reducing reflection losses. The central exhaust tube in the reactor is a spherical bulb to ensure a better overlap between the particle suspension volume and high flux density. Figure 2 shows a photograph of the solar simulator and the reactor vessel. A number of runs were made to observe the heating of particle-gas mixtures in the reactor. When the reactor was wrapped with insulation, temperatures in excess of 1200 K were reached.

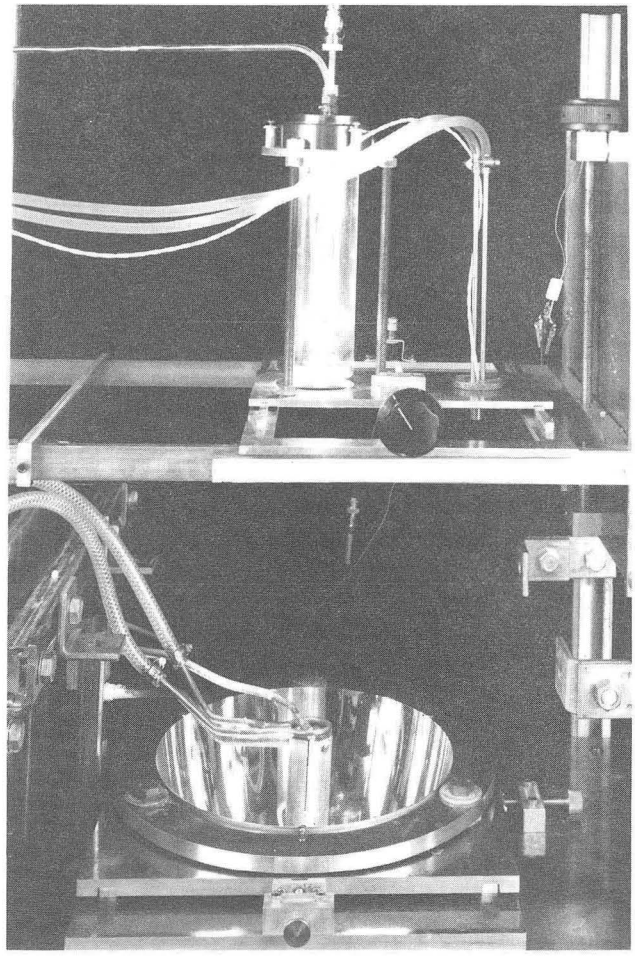

Figure 2. The Solar Thermal-Activated Radiant Reactor (STARR) in place at the focus of the arc-image solar simulator below it. (CBB 848-5990)

Work was completed on a mechanical shaker and cyclone chamber for entraining small particles in a gas stream. Commercially available powders of carbon, hematite, and magnetite were successfully entrained, and optical extinction measurements were performed on the particle suspensions. Extinction is defined as the fraction of the energy from a He/Ne laser removed from the laser beam after passing through a known length of the particle-gas mixture. The mass loading of the particles in the suspension was determined by drawing a known volume of the particle-gas mixture through a filter and weighing the filter. Samples were cut from the filter, and scanning electron micrographs were made to determine the particle size distribution. Hematite and magnetite were chosen because of their desirable optical properties and their possible roles as catalysts in a ther-

mal storage cycle and in a two-step water-splitting cycle, respectively.

In another application of radiantly heated small particle suspensions, we have undertaken preliminary studies of solar detoxification of hazardous chemical wastes. In FY 1984, we completed a successful experimental demonstration of the destruction of a surrogate for a refractory toxic chemical by the STARR reactor. The toxic wastes that are most resistant to destruction by incineration are the polychlorobiphenyls (PCBs). Dichlorobenzene was chosen as a surrogate for PCBs because it is considerably less toxic but has similar thermal decomposition properties. An injection system for introducing the hazardous waste material into the particle-gas stream was installed and tested. Results of tests using carbon particles as the absorbing material in air indicated that temperatures near 1200 K were reached and that the carbon particles were oxidized during passage through the reactor. After leaving the reactor, the gases were passed though an impinger for chemical analysis. An ion-selective electrode (ISE) was used to monitor the HCl content of the water from the impinger. The performance of the ISE was verified at concentrations expected from the experiment. Measurements with the ISE indicated that more than 90% of the dichlorobenzene was destroyed after passing through the reactor.

PLANNED ACTIVITIES FOR FY 1985

The research described above has enabled us to open up entirely new ground in the field of radiant-energy processing of fuels and chemicals. This research, along with the results of the successful solar test of the SPHER Mark I receiver, has established LBL in a leading role in the development and understanding of direct-absorption small-particle solar receivers. It is anticipated that in FY 1985 our research effort in direct-absorption receivers will be significantly expanded as part of the DOE Solar Fuels and Chemicals Program. The emphasis in FY 1985 will be on understanding heating rate effects, flow/process design, and further development of instrumentation.

A further outcome of FY 1984 research was the initiation of a project to investigate the feasibility of using directly heated small-particle suspensions to produce hydrogen. The particles would be used both as the absorber of solar radiation to heat the gas and as a catalytic site for chemical reactions. Plans call for purchasing a gas chromatograph to detect and quantify the reaction products.

Finally, since we have successfully demonstrated the capability of a small-particle heat-exchange receiver to destroy toxic waste materials, we plan further work to determine the conditions necessary to achieve the 99.999% destruction and removal efficiency required by the Environmental Protection Agency.

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