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Program Report for FY 1984 and 1985 Atmospheric and Geophysical Sciences Division of the Physics Department

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Program Report for FY 1984 and 1985 Atmospheric and Geophysical Sciences Division of the Physics Department

Abstract

This annual report for the Atmospheric and Geophysical Sciences Division (G-Division) summarizes the activities and highlights of the past three years, with emphasis on significant research findings in two major program areas: the Atmospheric Release Advisory Capability (ARAC), with its recent involvement in assessing the effects of the Chernobyl reactor accident, and new findings on the environmental consequences of nuclear war. The technical highlights of the many other research projects are also briefly reported, along with the Division's organization, budget, and publications.

Introduction

The Atmospheric and Geophysical Sciences Division (G-Division), and its precursor organizations, have contributed to the research and safety aspects of several major programs at the Lawrence Livermore National Laboratory (LLNL). Since the 1950s, these programs have included nuclear testing, the peaceful uses of nuclear explosives, basic studies in climate simulation, and health and environmental research. Since 1974, the responsibility for atmospheric research has been consolidated in G-Division, one of several research divisions within the Physics Department.

Since the Division's formation, core capabilities in the analysis of transport, diffusion, and deposition on local to global scales, coupled transport-kinetics modeling, radiation transfer in the atmosphere, and climate simulation have been used in assessment of several military and civilian environmental issues. These simulation capabilities and the issues investigated are summarized in Table 1. The most recent issues are on the emerging edge of environmental research: for example, the environmental consequences of nuclear war, the early detection of CO_2-induced warming of the Earth's climate system, and emergency response planning and assessment associated with major releases of toxic materials and radioactive materials. Over the last two years, two major projects have shown strong growth: (1) the Atmospheric Release Advisory Capability (ARAC) serving the emergency response needs of the Department of Energy (DOE) and the Department of Defense (DOD), and (2) research on the environmental consequences of nuclear war.

Some significant G-Program contributions are presented below:

- The prediction of radioactive fallout from near-surface and surface bursts from the local to global scales resulting from a large scale nuclear war.
- The development and implementation of ARAC, with the goal of determining a national center to serve the emergency response needs of DOE, DOD, and other federal agencies.
- The development, testing, and application of the Livermore regional photochemical air quality model (LIRAQ) used in development of the Air Quality Maintenance Plan for the San Francisco Bay Area and the study of inter-basin pollutant transport in northern California.

Table 1. Atmospheric science serving major environmental issues.

Scientific Area	Civil Issue	Military Issue
Local scale-transport, diffusion and deposition	Consequences of radioactive releases from a nuclear reactor	Fallout, rainout, self-induced rainout of nuclear aerosols
Regional scale-transport, diffusion, and deposition	Fate of pollutants in complex terrain	Fallout and exposure patterns for major releases for nuclear facilities/reactors
Continental scale, transport, diffusion, deposition and transformation	Acid rain, air corridor safety following high yield foreign weapons tests.	Diagnostic use of models to deduce nuclear source strengths; Southern Hemispheric detection capability
Stratospheric chemistry	Impact of CFMs and other trace gases on the ozonosphere	Impacts of strategic Exchange on ozonosphere
Climate system simulations, perturbed climate-state predictions	CO_2 effects on climate	Response of the Earth's climate system to soot, NO_x and Dust from strategic exchange
	Interactions of climate and energy	
	Early detection of the CO_2 climate signal	Co-authorship of ICSU study of the "Environmental Consequences of Nuclear War"

• The Division's lead role (FY 1979–FY 1985)* in the DOE Atmospheric Studies in Complex Terrain (ASCOT) program, whose goal is to predict the fate of pollutants released into terrain-dominated flows.

• An extensive research effort devoted to improving understanding of the phenomena of rainout and self-induced rainout from clouds generated by nuclear explosions, as well as scavenging of soot/smoke aerosols generated by post-war fires.

• The development of finite-element modeling (FEM) capabilities for hydrodynamics, transport-diffusion, and the simulation of terrain dominated flows.

• The development of models of coupled transport and chemical kinetics in the stratosphere, including representation of the several competing catalytic cycles, for assessment of fluorocarbon impacts and the effects of other trace gases.

• Studies of the potential impact on stratospheric ozone of high-altitude aircraft engine emissions, manmade chemicals, and large-scale nuclear war.

• Development of the first interactive global climate model treating the radiative interaction, transport, and scavenging of smoke from post-nuclear fires.

• Development of a zonally averaged global climate model (ZAM) that has evolved into the statistical dynamic climate model (LSDM) currently in use to assess the sensitivity of the climate system to perturbations by man (e.g., CO_2, Arctic soot) and nature (e.g., volcanoes).

• Modification of the Oregon State University (OSU) General Circulation Model (GCM) as part of a cooperative project with OSU and the State University of New York Stony Brook involving the intercomparison of climate models in an attempt to better understand their differing responses to increased atmospheric carbon dioxide.

A continuing theme of G-Division research has been the quest for more accurate methods of solution of the mathematical set of equations governing the regional and global scales being simulated. The solution methods should be sufficiently accurate that changes in the physics or

* FY means fiscal year, beginning each October.

boundary conditions, even if subtle, can survive extended integrations. Operating in this spirit, our advanced modeling team of the early 1970s developed the atmospheric-diffusion particle-in-cell code (ADPIC) and its companion regional diagnostic flow model (MATHEW). Subsequently, these models were tested, improved in operational speed, and now form the core of the real-time ARAC system. During the 1980s, our advanced modeling team has continued this quest for more accurate but affordable methods of solution. The current thrust is in the direction of finite-element methods (FEM) in geophysical hydrodynamics, with the initial applications being the simulation of liquid natural gas (LNG) spills in three dimensions and the calculation of nocturnal drainage flows for the ASCOT project, both of which involve density-driven flow over three-dimensional complex terrain. On the global scale, we have developed a Lagrangian Sampling Parcel (LSP) technique that can accurately represent the transport and disposal of injected materials.

The G-Division highlights of the past two years (FY 1984 and FY 1985) reflect a growing national and international involvement in assessment of current and major scientific questions. For example, about one-third of the U.S. research on "nuclear winter" is now being led or conducted by LLNL. Because of these studies our simulation capabilities of environmental systems have been increasing at a rapid rate. These include a new three-dimensional, compressible, nonhydrostatic hydrodynamics model for simulation of plume rise from massive urban fires and an improved, three-dimensional, climate simulation model that allows interaction between radiatively active aerosols and the evolving hydrodynamics, including suitable representation of scavenging of the soot clouds.

A second example has been the transfer of ARAC technology during the past several years to other countries such as Italy, Japan, and others. For instance, the United Kingdom has requested access to ARAC guidance in support of nuclear capabilities in their country. The most recent international involvement of ARAC has been to send a senior scientist to the Indian Science Congress in January 1986 to bring up-to-date information on emergency planning, response, and assessment in the wake of the Bhopal accident. Finally, two of our scientists served as senior coauthors (and three others as collaborating authors) of the SCOPE/ENUWAR study on *The Environmental Consequences of Nuclear War, Volume 1,* published by John Wiley in 1986.* In addition to being an 18-month effort to collect, synthesize, and seek consensus of the international scientific research, this study is probably the most comprehensive, complete, and balanced to date.

This year's report also covers research for the periods FY 1983 and FY 1984, for which formal annual reports were not prepared. During these years, a sizable research team was organized to investigate the environmental consequences of nuclear war. Further, these same years required strenuous management activity to resolve fiscal uncertainties while ARAC responded to increased DOD requirements. The research effort of investigating the environmental consequences of nuclear war is now stabilized and productive. The ARAC budgets for FY 1986 and 1987 are becoming firm, the staff and service are stabilized, and plans have been developed for modernizing the ARAC hardware in order to meet the DOE and DOD requirements more expeditiously and to provide high-quality crisis management advisory products.

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* SCOPE is the Scientific Committee on Problems in the Environment, formed under the auspices of ICSU (International Council of Scientific Unions). Their project, ENUWAR, assesses the environmental consequences of nuclear war. Michael MacCracken and Charles Shapiro were two of six principal authors of Volume I on Physical and Atmospheric Effects. Peter Connell, Ted Harvey, Sang-Wook Kang (of the Mechanical Engineering Department), and Kendall Peterson were four of the seven collaborating authors. George Bing, Joyce Penner, and Chuck Leith participated in workshops. Camera-ready copy for the book was prepared by the G-Division secretarial staff.

Organization

Our research program is organized into five broad themes: Advanced Modeling, Regional Modeling and Assessments, CO_2 and Climate Research, Atmospheric Radiation and Chemistry, and Special Projects. These five major themes encompass the major capabilities and expertise within the Division. Each theme is managed by the Division Leader, the Deputy Division leader, or an Associate Division Leader. Specific projects generally fall within a theme, but often cut across two or more themes. Leaders for specific projects are drawn from within the themes; while staff members may be leading one project, they also may be working with others on another project. This is consistent with the team-oriented approach to research that is encouraged within the Division. See Fig. 1 for a breakdown of the G-Division projects, sponsors, and principal investigators for the five research themes during FY 1986.

The G-Program has a staff of about 60, of whom 50 are professionals involved in research. Resources from other parts of the Laboratory such as Electronics Engineering, Physics, Numerical Analysis, and Computer Science are made available to the Division on a short-term or long-term basis, depending on project requirements. Presently, the Division receives support from seven other groups within the Laboratory. In addition, seven staff members of ARAC are provided by EG&G to support the operational mission of ARAC.

Regional Modeling and Assessments 25.5 FTE $5015 K M. Dickerson	Advanced Modeling 3.3 FTE $584 K P. Gresho	CO_2 Climate Research 15.7 FTE $3083 K M. MacCracken	Stratospheric Research and Radiation Transport 4.7 FTE $953 K F. Luther	Special Projects 12.7 FTE $800 K J. Knox
ARAC Base Program (DOE-ONS) M. Dickerson	Finite-Element Techniques (DOE-OHER) P. Gresho	CO_2 Climate Modeling (DOE-BES) M. MacCracken	Satellite Ozone Analysis Center (NASA) F. Luther	Radionuclide Studies (DOD-DNA) J. Knox
ARAC Operations Support (DOD-DNA) M. Dickerson	LGF Vapor-Dispersion Modeling (DOE-EP) S. Chan	CO_2/Climate Management (DOE-BES) M. MacCracken	Stratospheric Calculations (EPA) D. Wuebbles	Special Atmospheric Studies (LLNL Phys. IR&D) J. Knox
ASCOT Modeling and Remote Sensing (DOE-OHER) M. Dickerson	FEM Laser Isotope Separation (DOE-OMA) P. Gresho	Climate Model Intercomparison (DOE-BES) G. Potter	Transport Kinetics (NASA) D. Wuebbles	Panel Support (USAF) J. Knox
ASCOT Support (DOE-OHER) P. Gudiksen	3-D FEM (DOE-OMA) R. Lee	Environmental Consequences of Nuclear War (DOE-OMA) M. MacCracken	UARS (NASA) D. Wuebbles	Environmental Consequences of Nuclear War (DOE-ISA) J. Knox
ASCOT Measurements (DOE-OHER) P. Gudiksen		Environmental Consequences of Nuclear War (LLNL IR&D) M. MacCracken	Trace Gases (DOE-BES) D. Wuebbles	G-Program Administrative Support J. Knox
ARAC ARG Support (DOE-OMA) M. Dickerson		Environmental Consequences of Nuclear War Atmospheric Studies (DOD-DNA) J. Penner		
Regional Tracer Analysis (DOE-OMA) J. Knox/D. Rodriguez		Clouds/Radiation Interactions (DOE-BES) F. Luther		
LIRAQ Model Application (BAAQMD/ARB) J. Penner				

G-PROGRAM ADMINISTRATION

Joseph B. Knox, Division Leader
Michael C. MacCracken, Deputy Division Leader
Marvin H. Dickerson, Associate Division Leader
Philip M. Gresho, Associate Division Leader
Frederick M. Luther, Associate Division Leader
Floy L. Worden, Program Manager

Figure 1. G-Division projects, sponsors, and principal investigators for the five research themes in FY 1986.

Status Reports on Major Projects

Because of the two-year lapse in G-Division Annual Reports, we now present comprehensive status reports on the Atmospheric Release Advisory Capability, which serves the DOE and DOD emergency response, planning, and assessment needs, and the research program on the Environmental Consequences of Nuclear War (more popularly known as "Nuclear Winter"). Technical highlights are also presented for three selected projects that are sponsored by DOE and have strong potential for further development under the auspices of DOE and other governmental agencies. These projects are Regional Modeling, ASCOT, and CO_2 Effects Research.

Atmospheric Release Advisory Capability (ARAC)

Introduction

The Atmospheric Release Advisory Capability, which has been in existence for over eleven years, (Dickerson and Orphan, 1976; Dickerson, Knox, and Orphan, 1979; Dickerson, Gudiksen, and Sullivan, 1983), is a real-time emergency response system designed to assess the potential environmental consequences of radiological accidents. It responds to a wide spectrum of atmospheric releases that may be associated with transportation accidents or accidents at Department of Energy or Department of Defense nuclear-capable facilities as well as at nuclear power plants. The ARAC consists of communications and computer systems, data bases and verified atmospheric dispersion models, and an experienced assessment staff. During the mid-1970s we developed and tested a prototype operational system that permitted operations of 40 hours per week beginning in 1979. Following ARAC's response to the Three Mile Island (TMI) accident in March 1979, the purge of krypton from the TMI containment in July 1980, and the Titan II missile accident in Arkansas in September 1980, the Departments of Energy and Defense initiated expansion of ARAC services. This expansion included new hardware and software for the system, increased staff, additional facilities for housing staff and computers, and expanded operational hours. Since its inception in 1974, ARAC has responded to over 80 real events, potential events, and major exercises.

The staff presently includes 26 scientists and technicians. Their background, training, and experience ranges from transport and diffusion physics, weather forecasting, and health physics to electronics engineering and computer science. Approximately half of the staff is involved in operations while the remainder is devoted to computer systems development and maintenance and model research and development. The experience level of many staff members in the area of emergency response for nuclear accidents is based on participation in response to actual or potential releases and major exercises over the past seven years. In addition to developing and implementing an expanded system, staff members are continually involved in planning and executing major exercises, briefing various organizations, conducting classes on emergency response, and coordinating activities with several government agencies.

The remainder of this section describes the current status of the ARAC system, requirements for obtaining the service, the organizations related to the ARAC service, and future directions for the service. Even though the ARAC service is presently limited to radiological accidents, the fundamentals of the service as an emergency-response resource would be applicable to toxic chemical releases as well.

ARAC Emergency Response Operating System

The ARAC operating system integrates data acquisition, data analysis, data-basing and management functions, and atmospheric transport and diffusion models to enable the ARAC staff to produce real-time assessments of accidental atmospheric releases of radioactivity. In order to support the emergency preparedness plans at the DOD nuclear-capable sites, the DOE nuclear facilities, and the Nuclear Regulatory Commission, the current expansion includes significant upgrades in computational, communications, and data-basing facilities as well as increased staff. The goals of this expansion are to be able to:

- Support up to 100 nuclear facilities.
- Simultaneously handle two emergency responses.
- Provide timely response to an accident at a "nonfixed" location.
- Automate manual data processing functions.
- Provide complete computer backup for the ARAC center.

The ARAC has traditionally used the Lawrence Livermore National Laboratory's central computing facility and several minicomputers to perform a hazards assessment of a particular accident. The current configuration includes ARAC-dedicated computers which will be used to perform the assessments. Two dual-processor main computers are linked by means of a high-speed local-area communications network with three front-end communications processors, two gigabytes of shareable disk storage, and a telecopier. This system, the ARAC Emergency Response Operating System (AEROS), will be able to interact via commercial telephone lines with the data communications terminal situated at each on-land nuclear site and with the Air Force Global Weather Central (AFGWC) (Sullivan, 1984).

The initial installation of the AEROS hardware has been completed, and a major portion of the communications, graphics, and terrain and geographic data-base components have also been completed. We are currently developing extensive software to automate the data acquisition, validation, and data-basing processes for speed of operation and reliable and accurate assessment. We are devoting a major effort to transfer the atmospheric dispersion models from the LLNL computer center to the AEROS. A structured software methodology was employed to enable the development staff of 25 computer scientists, meteorologists, health physicists, and engineers to progress simultaneously on several parts of the system development effort (Baskett, 1984). This technique ensures that system requirements are satisfied and adequate documentation of the software will be available for future maintenance and upgrades.

An integral part of the ARAC system is the nuclear facility data communications system, hereafter referred to as the site system. It consists of a small professional computer equipped with three modems, a 10-megabyte hard disk, two floppy disk drives, color monitor, and printer. One of the modems is connected to the site meteorological tower, and the remaining two are used to communicate with the ARAC center: one for voice and the other for data transmissions (Lawver, 1984). The system's configuration is shown in Fig. 2. The principal purposes of the site system are to:

- Permit site personnel to transmit meteorological and source term data to the ARAC center.
- Receive and display ARAC assessments.
- Collect and display local meteorological data.
- Perform localized Gaussian dispersion model calculations.
- Transmit messages to and from the ARAC center.

The software for the recently completed site system provides automated processing and displays information during an emergency. It features several menu choices that lead the user to standardized forms for data entry and displays.

Assessment Methodology

Simulation is the active part of the ARAC project, i.e., the process of developing an assessment for an emergency, exercise, or scenario development that employs a summation of project elements, including:

1. The rapid acquisition of meteorological and source term data from the event site, meteorological data for the surrounding region from the AFGWC, and terrain information from the ARAC terrain data base.
2. Interpretation and quality-control checking of the data by means of computer-generated graphics (Walker and Weidhaas, 1984) that include pseudo three-dimensional terrain views (see Fig. 3).
3. Determination of key parameters, such as source term, atmospheric stability, mixing depth, and boundary layer depth.

Following these three steps, model calculations are initiated and graphical displays of wind fields and plume trajectories can aid the assessor in visualization and add to the quality control of the simulation. Finally, graphical displays of calculated dose contours and surface contamination levels overlaid on local area maps are produced for transmittal to the event site and appropriate emergency preparedness officials. Examples of ARAC products are described in the next section.

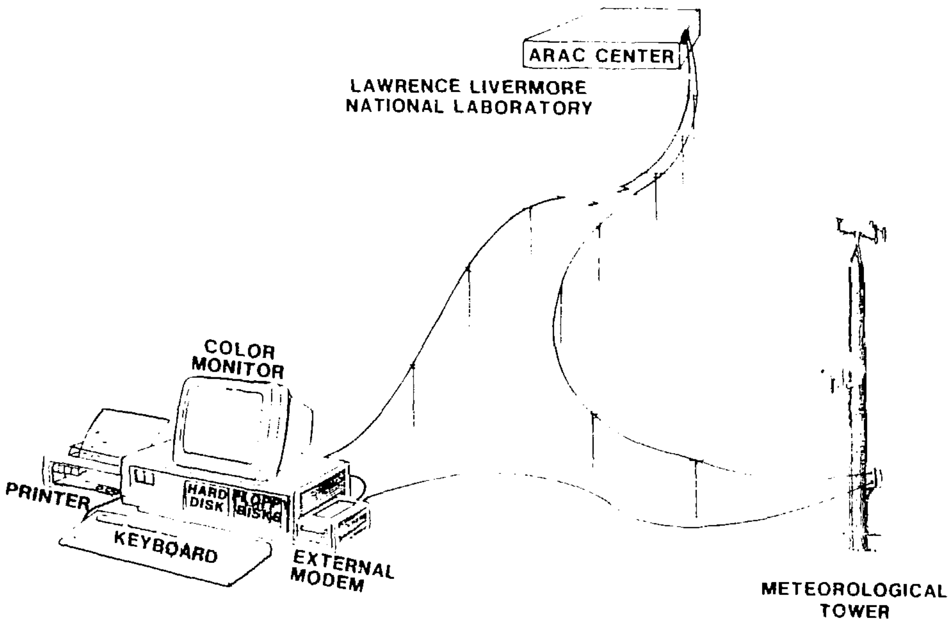


Figure 2. ARAC site system configuration.

One of ARAC's primary goals is to produce pertinent information in a timely and reliable manner for the emergency response manager. Thus, upon completion of the AEROS system and the hardware upgrade, an initial qualitative assessment based on several simplifying assumptions will be available within 15 minutes after notification. A complete assessment, based upon the initial input conditions, will be available within 45 minutes after notification of an event at the supported sites and within 90 minutes for any accident site within the continental U.S. Thereafter, ARAC will provide continuing support on an hourly basis until termination of the emergency. For nonsupported sites, very simple geographic background maps will be digitized in real time, whereas supported sites have the advantage of customized, detailed site maps. The graphical displays currently transmitted via high-speed telecopier will be replaced by the use of the ARAC site system.

ARAC Products

The ARAC products include graphical projections (contour patterns) of the location and levels of surface contamination and the potential radiation dose to people exposed to the resulting radioactive cloud. The initial radiological response force uses these projections to help assess the potential impact of the accident and to identify areas that the radiological survey teams will investigate.

Table 2 lists the atmospheric dispersion models that are presently used in the ARAC service. A brief description of each model is provided in the Summary of Modeling Capabilities section. The large scale global models 2BPUFF, a special version of PATRIC, and the KDFOC fallout model are used primarily for assessments associated with nuclear yields such as atmospheric tests of nuclear weapons. The MATHEW/ADPIC, PATRIC, and Gaussian (Continuous Point Source (CPS) and Instantaneous Point Source (IPS)) models are used for regional assessments, e.g., nuclear power plant accidents or nuclear weapons accidents involving the high-explosive dispersal of radioactive material. Because the MATHEW/ADPIC model is used for the majority of assessments, it will be used in this report to illustrate the ARAC products (Lange, 1984; Peterson and

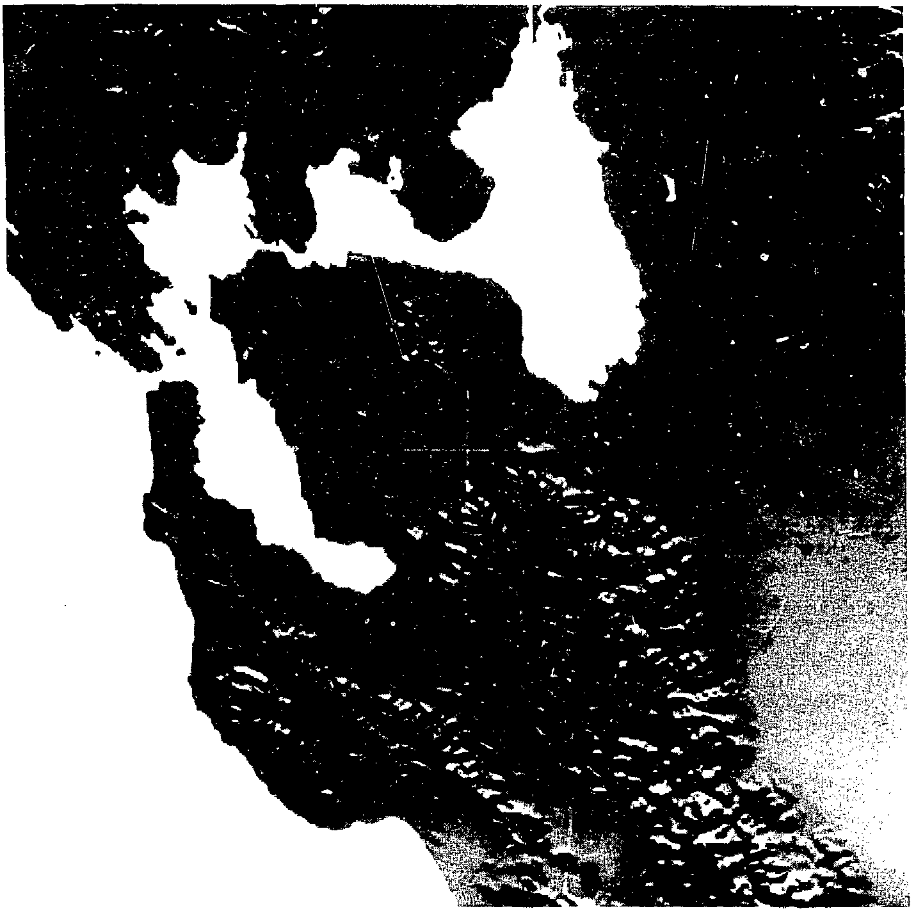


Figure 3. Graphical display of terrain data for the San Francisco Bay Area.

Lange, 1984; Rodriguez and Rosen, 1984) that may be generated in the unlikely event of a nuclear weapons accident at a military facility. We used a fictitious Air Force Base (Radnor) to simulate the following sequence of events:

1. Notification of the National Military Command Center (NMCC).
2. Notification of ARAC.
3. Initial Gaussian IPS calculation—available within 2–3 minutes from the site system.
4. Initial ARAC calculation—available from the ARAC center within 15 minutes after notification (contingent upon hardware upgrade).
5. Advanced ARAC calculation—available from the ARAC center within 45 minutes after notification.

Figure 4 illustrates the initial MATHEW/ADPIC calculation available to the Incident Response Force (IRF) on-scene commander from the ARAC center approximately 15 minutes after notification. This assessment assumes that all of the plutonium involved in the accident was aerosolized according to high-explosive detonation scenarios, which relate to an assessment

Table 2. ARAC operational dispersion models.

Model	Global Scale ~ 20,000 km	Synoptic Scale ~ 2,000 km	Regional Scale ~ 200 km	Meso Scale ~ 20 km
Simple	–	–	–	Gaussian
Intermediate	2BPUFF	2BPUFF	MATHEW/ADPIC KDFOC2	MATHEW/ADPIC KDFOC2
Complex	PATRIC	PATRIC	MATHEW/ADPIC	MATHEW/ADPIC

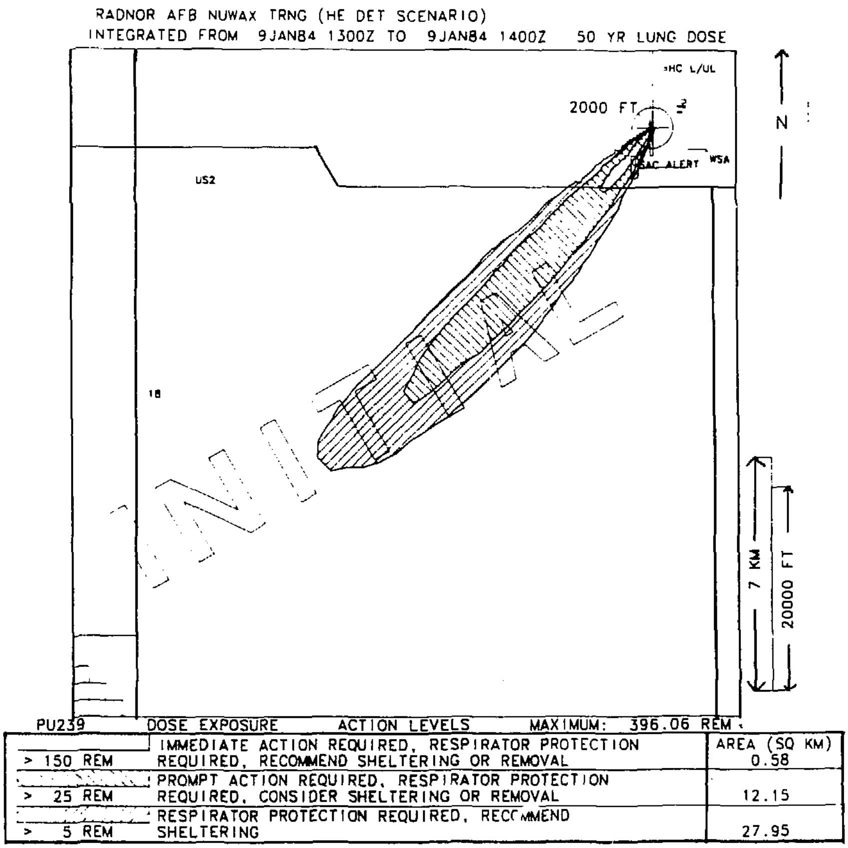
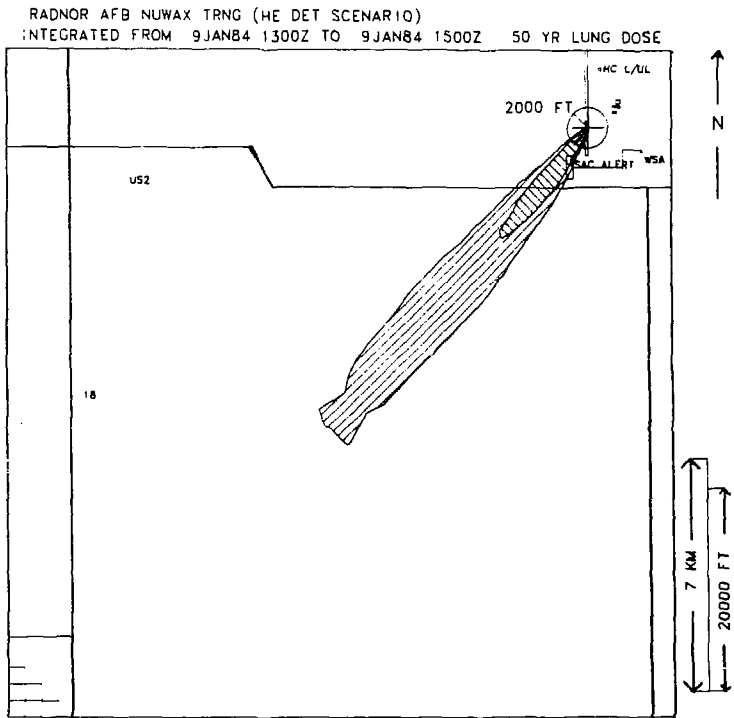


Figure 4. Initial MATHEW/ADPIC calculation available to the emergency-response manager in 15 minutes.



PU239 DOSE EXPOSURE ACTION LEVELS MAXIMUM: 182.93 REM

		AREA (SQ KM)
> 150 REM	IMMEDIATE ACTION REQUIRED, RESPIRATOR PROTECTION REQUIRED, RECOMMEND SHELTERING OR REMOVAL	0.02
> 25 REM	PROMPT ACTION REQUIRED, RESPIRATOR PROTECTION REQUIRED, CONSIDER SHELTERING OR REMOVAL	1.89
> 5 REM	RESPIRATOR PROTECTION REQUIRED, RECOMMEND SHELTERING	16.44

Figure 5. Complete MATHEW/ADPIC calculation for projected lung dose available to the emergency response manager in 45 minutes.

for a "maximum-credible" accident. This assessment does not explicitly include the effects of terrain but does retain the three-dimensional characteristics of the wind field. While performing the initial assessment, we are developing more complete meteorological and source term data bases for the advanced assessment, which is available to the IRF commander within 45 minutes after notification. This assessment, shown in Figs. 5 and 6, is based on the full capability of the MATHEW/ADPIC model. Additional assessments are produced (usually hourly) as long as needed. The projected lung dose due to the *inhalation of plutonium particles* by individuals exposed to the radioactive cloud (see Fig. 5) assist the IRF on-scene commander with evaluation of the potential hazard to the general public until comprehensive radiation measurements and bioassays can be performed. Action levels of 150, 25, 5, and 0.5 rem are used to provide general guidance for any protective actions that might be required. Figure 6 illustrates projected surface contamination levels that are used for establishing access to the contaminated areas and for clean-up if required. Action levels of 600, 60, 6, and 0.2 $\mu Ci/m^2$ are the general guidelines for ground contamination. Note also that the figures include a 2000-ft circle centered on the accident site. It denotes a generic high-explosives fragmentation radius. A distance scale is included on

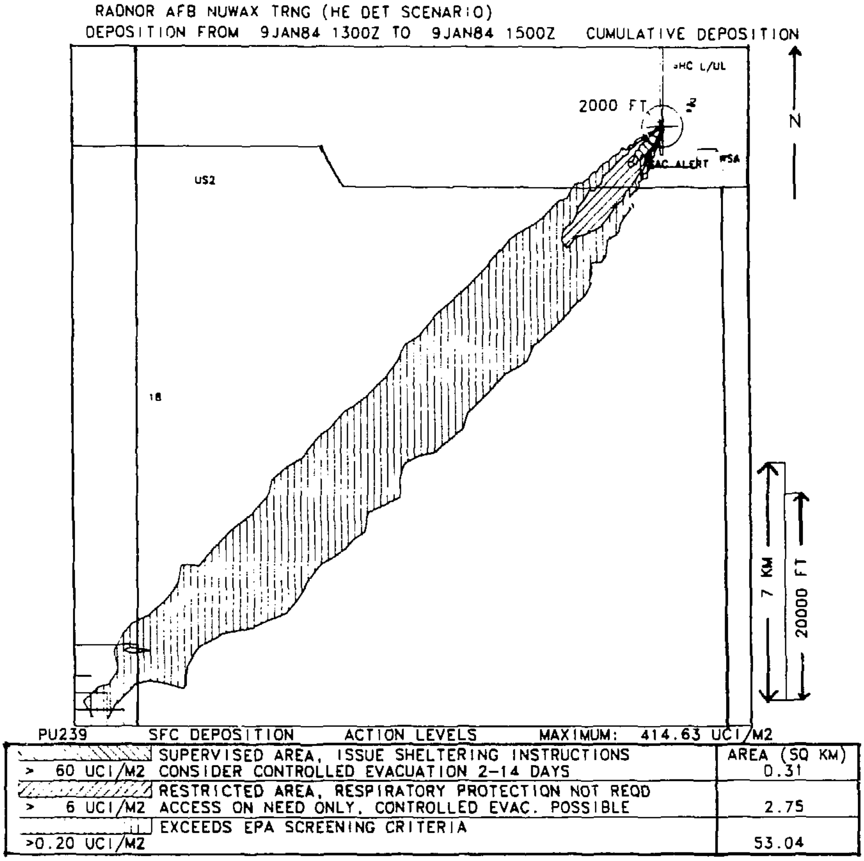


Figure 6. Complete MATHEW/ADPIC calculation for ground contamination available to the emergency response manager in 45 minutes.

the lower right side of the plot, and the squares situated in the lower left corner of the plot refer to the computational grid size that the ARAC assessor uses for quality control purposes.

These examples illustrate how the ARAC products have been tailored for the user. Assessments of incidents at DOE facilities or nuclear power plants have a different format and require a different interpretation. Experience gained by the ARAC staff over the past 11 years has shown that the assessment products need to be designed to meet the requirements of the users.

Requirements for Receiving the ARAC Service

To provide the ARAC services to a facility, several data bases must be prepared. Topographical and geographical information are required to establish the MATHEW/ADPIC model grid on which all the ARAC products are plotted. The standard ARAC site data base is a 200-km-square area centered on the facility of concern. The grid is divided into cells, each 0.5 km on a side. The terrain elevation of the bottom of each cell is obtained from the U.S. Geological Survey (USGS) digital terrain elevation data products. From this large grid

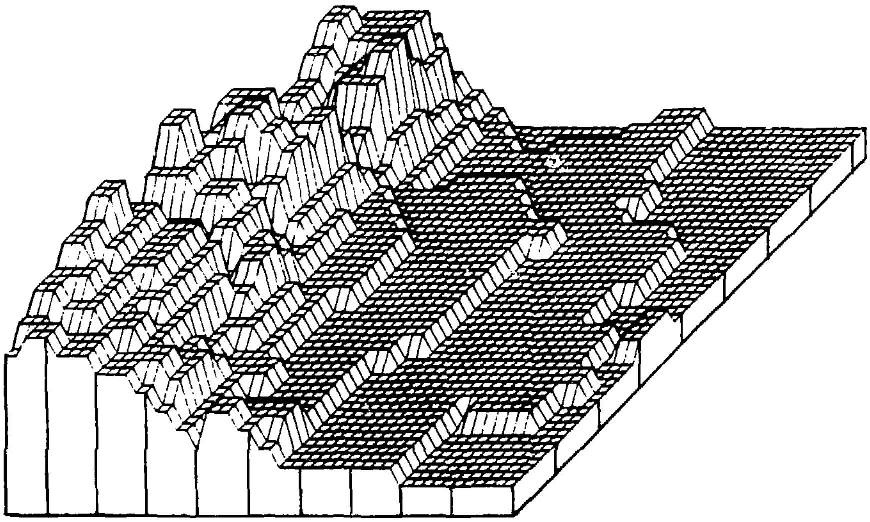


Figure 7. Example of cellular terrain structure used by the MATHEW/ADPIC model.

a model subgrid can be generated for any subregion of 40 × 40 cells. Figure 7 is an example of the cellular terrain structure on the bottom of the three-dimensional model grid. Terrain data for the continental U.S. is resident on the ARAC computer system at 0.5 km resolution. The geographical information (i.e., water bodies, rivers and streams, roads and railways, urban areas) and associated names are digitized from the USGS 1:250,000 base maps. More detailed features specific to the facility of concern are taken from local site maps. The geographic features are used for reference points and are displayed on all ARAC plots (see Figs. 4–6). Once the 200-by-200 km master data base is established, any smaller subgrid map may be selected for a particular assessment.

Information is also needed in regard to the facility's operations and handling activities, including the "most probable" and "maximum credible" accident scenarios. This is used to set up "default" model input parameter files. These default files include data related to potential source terms (types of material at risk, particle size distribution, potential release rates, emission geometry, i.e., release height and stack characteristics, if applicable) and possible accident locations. The location and type of meteorological data available in the immediate vicinity are also included. Whereas ARAC acquires weather data routinely from the AFGWC and the National Weather Service (NWS), additional data from air-quality management districts, nearby industries, or local airports may prove very useful during an accident.

For sites judged by the ARAC staff to be deficient in meteorological data coverage, a weather tower needs to be installed at the site. ARAC technicians provide assistance in siting and installing such a tower, but site personnel are responsible for its operation and maintenance. Towers may be located on or near buildings, as long as the wind flow is representative of the free air flow and is not significantly altered at the sensor height.

The key measurements used by the ARAC models are wind speed and wind direction. While just about any anemometer and wind vane may be used, ARAC has standardized the use of two systems: one manual and one automated. These systems were chosen because of their sensitive response to low winds, durability, and cost effectiveness. The manual system (Fig. 8) provides a digital display of date and time, wind speed and direction, indoor and outdoor temperature, and barometric pressure. The measurements are automatically updated on the display once per minute. All values are instantaneous except wind speed, which is averaged over each minute. In order for ARAC to use these data

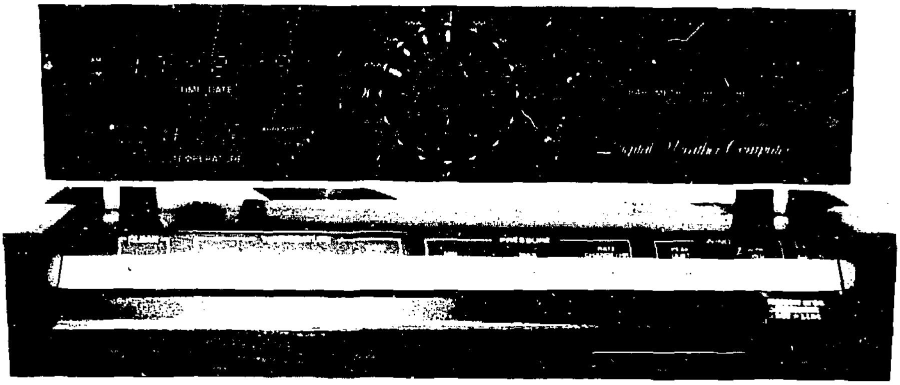


Figure 8. Supplemental meteorological data acquisition system.

in an accident situation, they must be read from the display and manually entered into the ARAC site system or called to the ARAC center over the telephone.

The automated meteorological data-acquisition system collects 15-minute-averaged wind velocity and temperature data in a microprocessor at the base of a 10-m tower (Fig. 9). It has two computer telephone modems: one is connected to the site system, and the other may be accessed directly from the ARAC center for redundancy. The site system is capable of collecting meteorological data in real time from up to nine levels on each of three separate towers. The standard installation records wind speed, wind gust, wind direction, temperature, and standard deviation of wind direction on each tower level. The 10-m, single-measurements-level tower, shown in Fig. 9 costs about $8,000 plus installation costs.

Training is provided for the site emergency preparedness personnel in order to help them operate the site system and use the ARAC assessments during an emergency. The ARAC staff periodically conducts a two-day training course that provides the foundation and fundamentals of the service. Trainees receive instructions on how an ARAC assessment is made, practice working with ARAC on an example accident (both with and without the use of the site system), and guidance through the interpretation of the ARAC model products. This course is only the beginning of the training program, as ARAC routinely participates in exercises at numerous facilities in order to keep the ARAC services vital and available for an immediate and efficient response.

Organizations Receiving ARAC Services

Four federal agencies presently receive direct emergency response support from ARAC, and six states have worked with the ARAC service on accidents, exercises, and joint participation projects. Two federal agencies, DOE and DOD Defense Nuclear Agency (DNA), are the major users of the service.

The DOE has provided funds for the initial ARAC development and operations for the past 11 years. The service is used for many offices of the Department that deal with radioactive material. These offices include:

- Facilities at Lawrence Livermore National Laboratory, Sandia National Laboratory (Livermore), Savannah River Plant, Mound Facility, Rocky Flats Plant, and Pantex. Additional facilities are expected in the future.
- Nuclear Emergency Search Team (NEST).
- Accident Response Group (ARG).
- Joint Nuclear Accident Coordinating Center (JNACC).
- Emergency Operations Center (EOC).
- Radiological Assistance Protection (RAP) Offices.

The DOD has largely funded the present expansion of the system and facilities to provide the ARAC service to the following organizations:

- Facilities at approximately 44 nuclear-capable facilities.
- Major Armed Services Commands.
- National Military Command Center (NMCC).

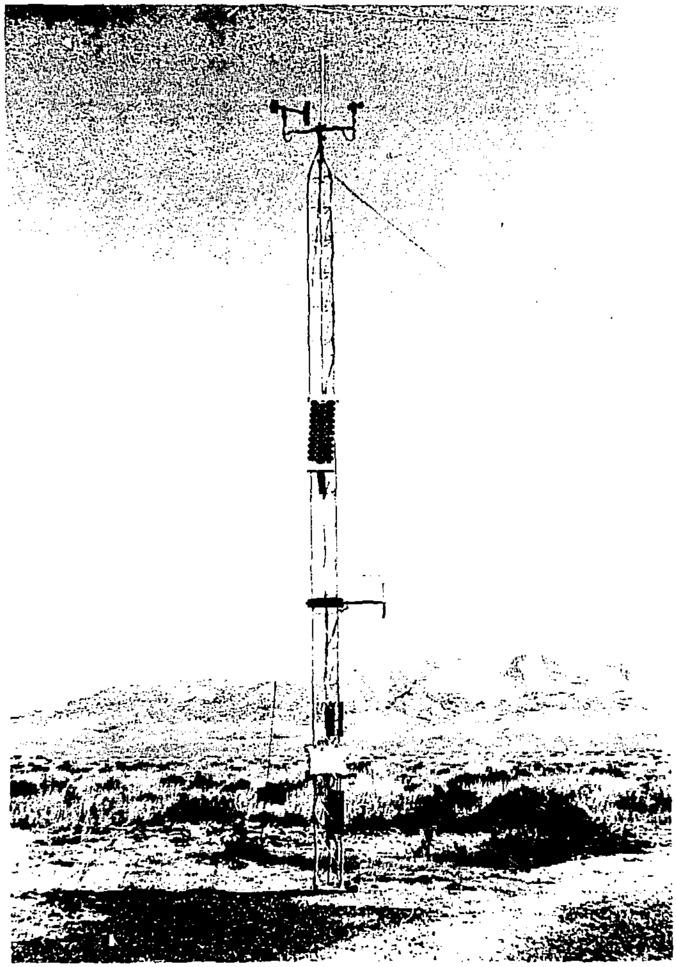


Figure 9. Automated meteorological measurements system.

• Joint Nuclear Accident Coordinating Center (JNACC).

The Federal Aviation Administration (FAA) has used the ARAC service to assess the potential radiation doses to passengers and crews of aircraft flying in or near airborne radioactive material. Originally the service was used in the event of Chinese nuclear weapons tests in the atmosphere; however, ARAC advisories were also issued to the FAA during the TMI accident for aircraft flying in and out of the Harrisburg airport.

The Nuclear Regulatory Commission requested and used the ARAC service as an emergency response resource in a major federal field exercise. Since this exercise, plans have evolved to include the ARAC service as a resource for the Nuclear Regulatory Commission for accidents involving civilian nuclear facilities. For example, they recently called for ARAC's assistance during the release of SF_6 from a nuclear facility located in Gore, Oklahoma.

The ARAC has worked with the states of New York, California, Pennsylvania, Virginia, Florida, and Texas. A continuing cooperative venture with New York State has resulted in the transfer of selected ARAC models to its computer system (Gotham, Krawchuck, and Matusek, 1985; Krawchuk, Grotham, and Matusek, 1985). Most work with the other states has been associated with joint involvement in exercise planning and execution, an activity that is expected to increase in the future.

In addition to providing an emergency response service to U.S. government agencies, the ARAC staff has worked with scientists from several foreign countries to help them develop emer gency response plans. This work has included the transfer of the ARAC computer modeling and accident-response-system technology and cooperation on studies of mutual interest. The Italian Ente Nazionale Energie Alternative (ENEA) began working with ARAC personnel in the early 1980s to move the MATHEW/ADPIC computer codes to their emergency response computer system. Since that time, an ongoing cooperative research and technology exchange program has continued at a moderate level (Gudiksen et al., 1983, and Dickerson and Caracciolo, 1986). The Japan Atomic Energy Research Institute implemented these computer codes on their emergency response system in 1982 (Asai et al., 1982). The Swedish National Defense Research Institute moved the codes to one of their facilities in 1983. More recently, the Korean Advanced Energy Research Institute has received copies of these computer codes and is installing them on their computer system. Other studies are ongoing with the United Kingdom, Israel, and Spain.

Future Directions

In the operations area, sites are being added to the system this year and personnel from each site will attend training courses at LLNL. Exercise participation will continue with the sites and with DOE and DNA headquarters, as will installation of site computer systems and meteorological towers. For the remainder of 1985, the major systems development effort will be focused on transferring the MATHEW/ADPIC models from the LLNL computer center to the ARAC computers. This task, expected to be completed during FY 1986, will permit the ARAC operations staff to become much more involved in exercise participation with each site without causing a severe impact on the LLNL computer center.

The AEROS is capable of being expanded as needs arise. New data bases can be developed to increase the responsiveness and quality of the system. Now a substantial effort is being invested in the development of a continental-scale geographic or base-map data base to match the existing topographic data base. In the future, comparable demographic and land use data bases will be required, particularly as chemical accidents ascend to higher levels of importance with responsible government agencies. Extensive radiological dose conversion-factor data bases are also in the process of development for both the external and internal dose pathways. Comparable data bases need to be developed for the chemical/toxic materials hazards area. Future applications of ARAC may range from biological substance releases to dust clouds produced by volcanic eruptions. Thus, the long range goal of ARAC is to provide a national capability for emergency response to a wide range of potential accidental releases of hazardous materials into the atmosphere.

Research will begin on the development of operational time-dependent models for forecasting the wind and temperature fields on the scale of 100 to 200 km. The models will be used to forecast consequences in time ranging from 6–12 h. The models will be used in conjunction with the existing MATHEW model to improve the ARAC capability to assist emergency-response managers plan protective measures for long-term events or events that involve the incipient release of hazardous materials.

ARAC Response to Chernobyl Reactor Accident

On April 26, 1986, a nuclear rector at the Chernobyl energy complex, near Kiev in the U.S.S.R., suffered a major accident. Two days later, fission products were detected in Sweden and Finland. It was later confirmed by the Soviet Union that an accident had, in fact, occurred.

Once the magnitude of the accident began to unfold and the time of the accident initiation was estimated as 00Z G.m.t. April 26, 1986, it was apparent that ARAC had the necessary resources and capabilities to respond to the accident; however, these capabilities were not interfaced to provide a realtime assessment of potential impacts on public health on a space scale of 2000 to 3000 km for a surface release. Once meteorological data were received from the AFGWC, we calculated normalized air concentration and ground deposition of I-131 and Cs-137 for Scandinavia. These calculations were used in conjunction with measurements of I-131 and Cs-137 taken in Scandinavia to estimate that approximately 50% of the volatile radionuclides were released in a surface cloud over a period of several days. We also estimated, based on measurements and comparison with the Windscale accident in 1957, that less than 1% of the refractories escaped from the reactor.

An upper level cloud, based on the initial explosion and fire, was established between 800–4200 m in the vertical. This cloud contained the fission material that was detected first by I-131 measurements in rainwater in Japan within a week of the accident initiation and 3 days later in the western U.S. Measurements of I-131 in milk in the U.S. were within factors of 2 to 3 to our calculations. These measured values were over an order of magnitude below the lowest Food and Drug Administration protective action guideline for milk.

Figure 10 shows I-131 inhalation dose estimates for adults after 48 hours for eastern Europe and Scandinavia based on the estimated low-level, four-day source term for I-131, i.e., 36.8 x 10^6 curies. The two main branches of the cloud moved first toward Scandinavia during the first two days and also over Poland toward northern Italy during the next two days. Later estimates show the material also moving southward over Kiev toward Romania, with additional material moving to the east of Chernobyl. Our dose estimates show no serious consequences outside of the Soviet Union, with the possible exception of northeastern Poland. A more complete report describing the early ARAC response is in progress ("ARAC Response to the Chernobyl Reactor Accident," Dickerson et al.). In the future, we plan to expand our calculations to western Europe and also calculate the close-in dose with more resolution in the concentration field.

Environmental Consequences of Nuclear War

Introduction

The LLNL study of the environmental consequences of nuclear war is a multi-divisional effort of several tasks, ranging from source emissions to atmospheric sciences to biological and ecological effects. Staff to develop estimates of the regions and fuels affected by the nuclear explosions and fires are drawn from the Mechanical Engineering Department (S. W. Kang, T. Reitter), the office of the Associate Director at Large (G. Bing), and DNA staff on assignment at LLNL (R. Wittler). Study of the biological and ecological effects is performed by the Environmental Sciences Division (L. Anspaugh, J. Kercher). Description of these aspects, although not atmospheric sciences, are included in this report to provide a more comprehensive picture of LLNL research in this area and because G-Division staff participate in coordinating the entire program.

In the following sub-sections, significant questions in each area are first described, and then the status of research on them and the remaining questions are summarized.

Research Reports by Task

Scenarios and Targets. The goal of this task is to develop the ability to consider specific scenarios in order to estimate the amount of fuel that might be subjected to fires for any given scenario. Most previous estimates of smoke emissions have been developed without consideration of a detailed list of plausible targets and their co-location with potential fuel (i.e., cities, fuel storage areas, etc.). Instead, for example, it has simply been argued that a significant number of military targets will be located within or near cities, and that, therefore, a significant number of cities will burn. Estimates of average fuel loadings have then been used to generate estimates of smoke production. We are analyzing whether this procedure is appropriate. If, for example, many of the plausible targets are close together, the area subjected to burning would be reduced by overlap of the initially ignited area from each explosion. Also, some targets may be close to high fuel-load areas if they are next to a major city, whereas others might be located in areas in which the fuel load is below the average (e.g., along rivers and bays).

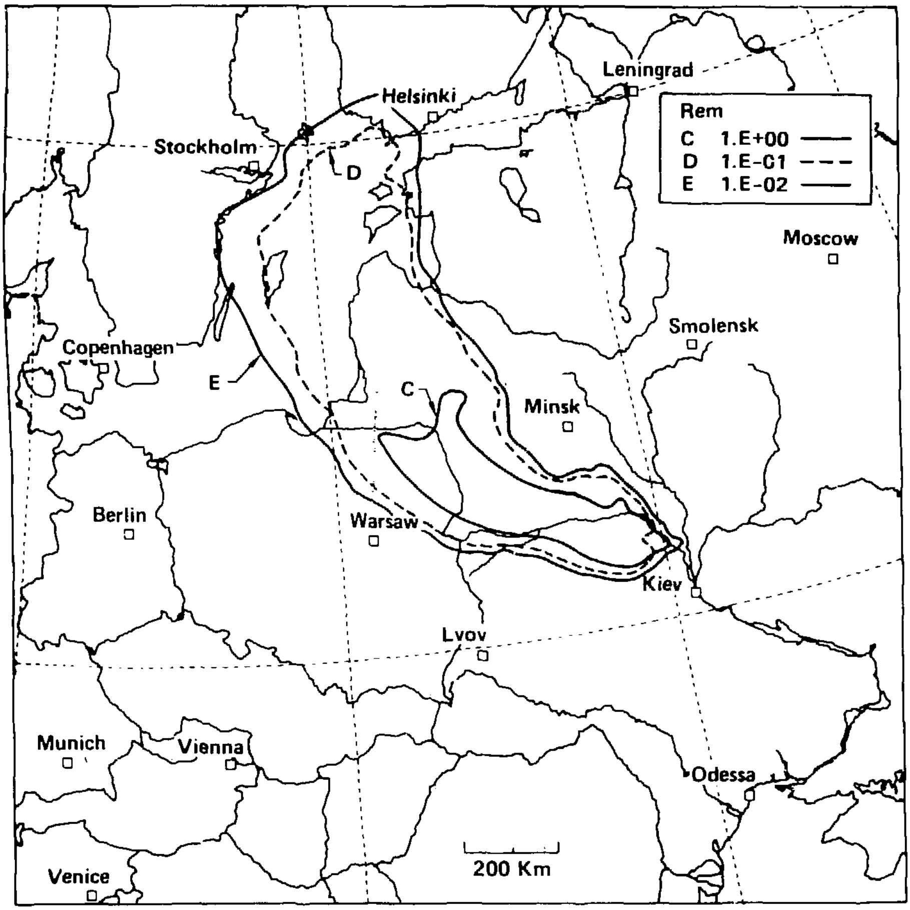


Figure 10. Estimated adult thyroid I-131 inhalation dose, 00 G.m.t., April 28, 1986, 48 hours after the beginning of the Chernobyl accident.

Last year, we developed the computer software necessary to calculate a nuclear scenario that associates targets with specific urban areas subject to fire ignition. We have also obtained a population data base for the United States. We expect to receive a data base that assigns fuel loading by target category for selected target types. We will use them to study the relationship of population density to distributed fuel loading (e.g., residential and commercial structures), which would provide a capability for developing estimates of the fuel subject to burning for particular scenarios. On a longer time scale, we hope to use existing climatological data to allow us to consider the likelihood of clouds and precipitation near targets and their potential effect on ignition fluence area.

Analysis of Fuel Load Available to Burn. We have examined a variety of sources to try to bound the estimates of the total amount of fuel available to burn in a typical city area. This analysis has led us to believe that estimates of fuel loadings from civil defense studies done in the 1960s may be too low by a factor of two. Our analysis will be checked by work that we are supporting at the University of California at Santa Barbara.

More importantly, however, we have looked at the total amount of fuel available in potential combatant nations. We have just completed a study that provides estimates of the total combustible material in all residential and nonresidential buildings in the 23 North Atlantic Treaty Organization (NATO) and Warsaw Pact (WP) countries. Separate estimates for the NATO and WP are included of asphalt in roofs and paving and of accumulations of plastics, synthetic fibers, and rubber in tires. Estimates of vulnerable crude oil and liquid petroleum product stocks have also been made. Total combustibles, not including wildland and agricultural fuels, are estimated to be approximately 7,700 teragrams (7.7×10^{15} g) of which about 1,300 teragrams are petroleum or petroleum-derived products. This total combustible inventory is one-half or less of the implied total combustible inventories in other recent studies. If *all* of the material were exposed to nuclear war ignition conditions, from 70 to 200 teragrams of smoke could be injected into the atmosphere, assuming the same smoke generation parameters used in other studies. The amount of smoke produced in a "realistic" nuclear war would be substantially less.

Fire-Initiation and Spread. The goal of this research is to define, for a few specific urban areas, how much fuel might be subjected to fire for specific targets and scenarios. We want to know, for example, if fire-spread might be significantly curtailed if sufficiently large firebreaks were present. An additional goal is to define the time history of heat release rates, so that they could be used to calculate injection heights for smoke as determined in the large-scale dynamics associated with the fire (See section entitled "Fire-Plume Dynamics: Injection Height of Smoke," below.)

During FY1984, we obtained a code that treats many of these processes. Studies were first performed for a uniform-city in which all tracts and all buildings were identically spaced and had uniform fuel loadings. The code was analyzed for its sensitivity to variations in input parameters. This year, we have applied the code to study the possible behavior of fires that could result from attacks on San Jose, California, and Detroit, Michigan. These cities were chosen because fuel load distributions were available from studies in 1968. Figure 11 shows the areas initially affected by fire and after 5 hours and 25 hours for San Jose. Because many vacant tracts occur within the San Jose and Detroit grid areas, much smaller amounts of total fuel are "burned" in both Detroit and San Jose than in simulations for the uniform city. We also found that the specific fuel loads per household in the 1968 studies appear to be a factor of two less than those computed using an inventory method (see section entitled "Analysis of Fuel Load Available to Burn," above.)

The results tend to show that for many target locations after 24 hours the fuel burned would be within 25% of the total amount of fuel within the initially ignited and debris area. However, our simulations in Detroit showed that when the initially ignited area was next to the center of the city, the total fuel consumed after 24 hours was about double that in the initially ignited and debris area. These results indicate that improving the estimates of total fuel burned in a major nuclear war will require study of specific target sets and their location with respect to fuel load distributions.

The peak fire intensity is a much more complex function of fuel load. Fire intensity varies in a non-linear manner with building density, for example, because of the dependence of the rate of fire spread on building density. The range of fire intensities computed for simulation of San Jose and Detroit is close to the range of intensities considered in our fire plume studies (see section entitled "Fire-Plume Dynamics: Injection Height of Smoke," below). Our estimates so far do not include an estimate for the rate of burning of the debris area associated with each nuclear explosion.

Most of the results produced so far have assumed that fire/wind interaction and firefighting efforts can be ignored. If this is the case, significant spread of the fire is possible. A simple calculation has been done to estimate the limitation to fire spread when inward-flowing fire wind speeds are larger than ambient values. For the uniform city case, the total fuel burned after 24

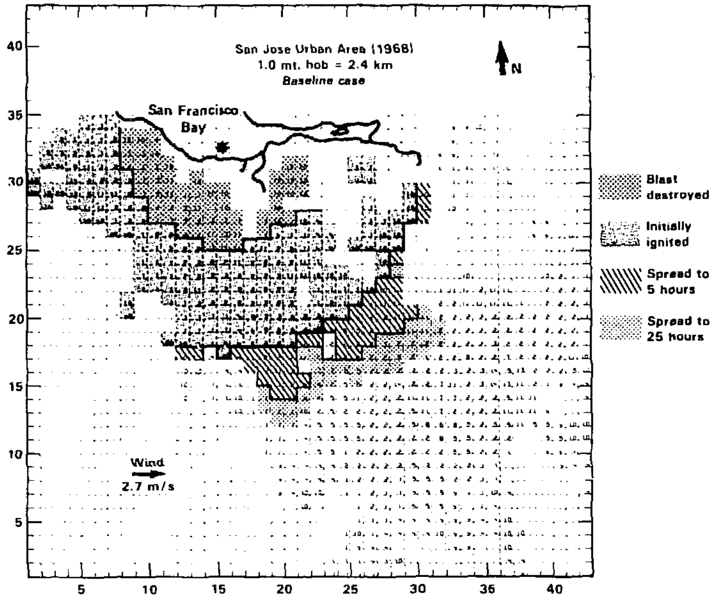


Figure 11. Areas affected by fires and blast following a 1-MT nuclear explosion near San Jose (assuming 1968 development).

hours was only decreased by about 20%, because the tracts involved burned more thoroughly than without fire and wind interaction. More work is needed to identify those situations that produce winds greater than ambient. For example, such winds would be expected if the fuel involved were greater than the 13 Tg of fuel associated with a direct hit on downtown Detroit.

Fire-Plume Dynamics: Injection Height of Smoke. The goal of this research is to determine the injection height of smoke. Originally, this was thought to be extremely important because low-level smoke injections have less climatic impact than higher level injections. For a summertime injection, however, global climate models have indicated that solar heating of the smoke can, under some conditions, cause lofting of the smoke from even low levels, so injection height may be a less critical parameter. The height of injection may be important, however, on shorter timescales appropriate to mixing the smoke over mesoscale regions in cold seasons and when there are also large dust injections into the stratosphere.

During FY 1984, we applied an existing Laboratory code to this issue. We found smoke injection heights depend on heat release rates and background atmospheric conditions of temperature lapse rate, wind speeds, and moisture content. This year, we improved the turbulence model in this code by adding a term that describes the effect of buoyancy on turbulence. We compared the predictions of the code to observations of both the Hamburg, Germany, firestorm and a smaller intensity fire that occurred in Long Beach, California. Figure 12 shows the results of the Hamburg simulation. Our results compare favorably to the observations over the wide range of intensities represented by the Hamburg and Long Beach fires. Further work is necessary to verify the code's behavior when condensation is a factor in determining injection heights.

We investigated several fire intensities and compared them to the injection heights assumed by Turco et al. (1983). We found relatively little injection at stratospheric altitudes even for very intense fires. This conclusion differs from that of other modelers who have found, under relatively low stability conditions, that up to 50% of the smoke may be injected into the stratosphere.

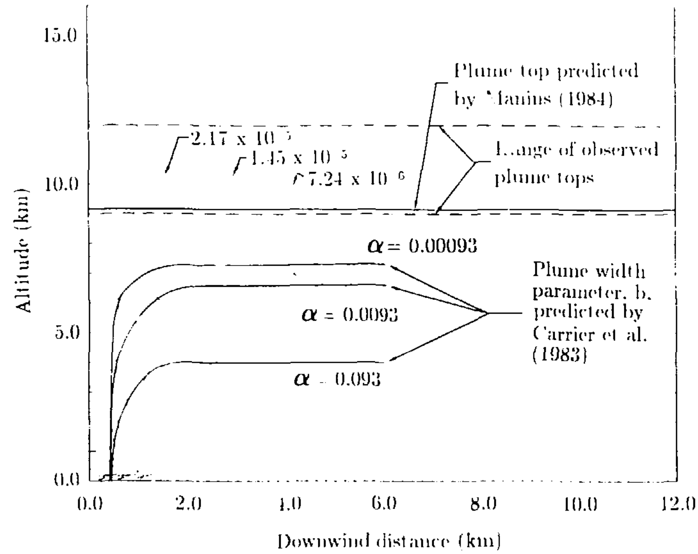


Figure 12. Smoke mass mixing ratios for Hamburg fire.

Further work is needed to clarify the reasons for this difference. Additionally, we found that large amounts of condensed water form above the most intense fires.

Since the code we have used does not predict the coalescence of condensed water droplets into precipitation, we cannot yet examine the effects of precipitation on dynamics or smoke scavenging. To address these issues, we have adopted a two-dimensional code, constructed by Mike Bradley as part of his dissertation at the University of Illinois (Bradley, 1985), that already contains precipitation physics. This code has been compared to known analytic solutions for both linear and nonlinear mountain waves and has been tested against cloud and thunderstorm events that are similar to the scale of interest for smoke plumes. A species equation for smoke and a surface-based source of heat, smoke, and water vapor have been added to this model. We are now in the process of testing this code to compare its predictions to those of the first code described above. Next, we will add parameterizations to describe scavenging and rainout of smoke particles.

We have also established a cooperative project to obtain a three-dimensional cloud-physics code. This code, which was developed by Klemp [of the National Center for Atmospheric Research (NCAR)] and Wilhemson (University of Illinois dissertation advisor of Mike Bradley), is widely accepted as a state-of-the-art numerical cloud model. We will be transferring this code to the Laboratory's computers, testing it, and adding a species equation for smoke. Scavenging parameterizations that are developed for the two-dimensional code should be readily transferable to this three-dimensional version.

The possibility of rapid scavenging of smoke in the early fire plume stage appears to be the most significant uncertainty for this scale, because results from interactive climate-smoke models now show that rapid heating of the smoke may lift it to high altitudes, even for smoke originally injected at low levels. More work is needed to confirm the lofting prediction, however, since infrared emission (and subsequent cooling) of dense patches of smoke may be able to limit lofting of it into the stratosphere.

Microphysics of Smoke. The goal of this research is to examine the effects of microphysical processes (i.e., coagulation and interaction of smoke with water) on smoke optical properties and lifetime. During FY 1984, we developed a code to calculate changing size distributions of smoke particles due to coagulation. Initial studies showed that significant changes in optical properties due to coagulation within the early plume were not expected. However, we found that, on time scales appropriate to the global scale, coagulation could significantly alter both the size distribution and optical characteristics of the smoke aerosols (assuming spherical particles). This work has been extended this year to examine the continuous effects of coagulation on scales from the initial fire plume to the mesoscale and global scale. A variety of cases have been modeled to examine the effects of different initial size distributions and absorption characteristics. For highly absorbing smoke (i.e., characterized by a refractive index of 1.75–0.3 i), the smoke optical absorption coefficient decreases to about 70% of what Turco et al. (1983) assumed would occur in 10 days. This coefficient (about 2 m^2/g) is similar to that recommended in the 1985 National Research Council report. For less absorbing smoke (refractive index equal to 1.53–0.05 i), the absorption coefficient after 10 days is close to 1.2 m^2/g—less than the recommendation in the 1985 National Research Council report. There is a need to examine whether these predictions are really appropriate for smoke—it may be that most of the carbon within the smoke remains in the form of branched chains of agglomerated smaller spheres. In this case, the absorption behavior may be more like that of the smaller individual spheres than like a single large sphere (see section on optical properties). Experiments in large fires are being planned by the national research program to help define the optical characteristics of the smoke, if properly conducted.

We have also looked at smoke coagulation that might occur as the result of larger debris swept up in the plume by the high winds associated with firestorms. Our study showed that if dust and debris concentrations were as high as expected in dust storms, rapid coagulation might take place. Optical extinction of the smoke under these conditions could decrease by about a factor of two as the smaller particles become attached to the micron-sized debris particles that tend to be rapidly removed from the atmosphere. The existence of such high concentrations of debris particles is speculative, however. Their concentration would depend on the type of surface debris that might form after the explosion and its interaction with the wind. If high concentrations of dust and other materials are lofted, significant coagulation would be expected in the fraction of fires that might become firestorms.

We have started to develop a code that couples coagulation of smoke particles, warm-rain microphysics, and scavenging of smoke. One mechanism for smoke removal, neglected in previous studies, is the incorporation of smoke into raindrops by nucleation-scavenging. This mechanism involves water condensing on the smoke particle itself. The degree to which this occurs depends on the size of the particle, its shape, its chemical composition, and the level of supersaturation reached in a rising air parcel. We have just started to use this code to examine the data from part of our contract with Desert Research Institute (DRI). The DRI has measured significant quantities of condensation nuclei in smokes produced in their laboratory. We will need to couple this model to a plume-code in order to realistically examine scavenging. However, we have found that if small supersaturations are reached within the rising plume and if smoke has at least some soluble material associated with it, approximately 50% of the aerosol particles and 90% of their mass will be incorporated into cloud droplets. Further study is needed to examine whether rain would develop and carry the particles to the surface.

The DRI is examining the ability of smoke particles from a variety of fuels to act as condensation nuclei. During FY 1985, they developed a procedure to make smoke from an acetylene source, an oil fire source, and a paraffin source. They also examined evaporated oil and paraffin and reported initial results in March 1985. The results showed significant numbers of cloud condensation nuclei from smokes (e.g., acetylene) that originally were thought to be hydrophobic. Since that time, they have concentrated their effort on developing procedures to allow aging of smoke in their large cloud chambers and on developing instrumentation to measure size-segregated cloud condensation nuclei. This latter measurement would allow us to determine whether particles act as cloud condensation nuclei because of their large size or because they contain soluble components.

Optical Properties of Smoke. During FY 1984, we calculated the range of smoke optical properties that would result from a range of assumptions about the radiative characteristics of smoke particles. We continue to review literature concerned with the optical properties of nonspherical particles and sooty particles. There is a need to evaluate the radiative properties of aggregates of particles of different optical characteristics because some smoke particles are primarily branch-chained aggregates of smaller solid particles while others are droplets containing graphitic carbon, organic carbon, and other material. We are coupling work in this area to work in experimental programs to obtain data about the composition and structure of particles from actual fires. It is expected that the DNA will support the necessary experimental fire research and that LLNL will provide guidance about which experiments would be most useful and relevant. With Sandia Laboratories, we are working on design of measurements for an experimental fire. They conducted an initial oil pool fire experiment in February 1986; another experiment is planned for August 1986. These should provide crucial data, because refinery fires may be a significant source of sooty, light-absorbing smoke.

There is also a need to develop computationally efficient subroutines that can account for the change in radiative properties of smoke as the particles evolve in time. Current computations are limited because they assume the optical properties of the small and large particles within our GRANTOUR/OSU model do not change from their originally specified values. The effect of changes in size distributions within these two particle-size bins need to be accounted for. In addition, efficient subroutines are needed to account for the infrared properties of smoke and for the changes in cloud properties as smoke becomes incorporated into cloud drops.

Meso-Scale Interactions. The goal of this research is to examine the interactions of dynamics, smoke, and precipitation during the first few days following the fires. We have studied one hypothesis, of stormy conditions developing especially off the east coasts of continents to cause early removal of the smoke. We have been examining this issue in a rather crude way that still allows some insight into the problem. Using an already developed sea breeze model, we turned off the Sun in order to simulate blocking of solar radiation by the smoke. During the first two days, the land surface inland of the ocean boundary cooled by more than 10°F, but the cooling was confined to a layer that was only about 100 m thick. Longer analysis times are necessary to extend the cooling to thicker layers, because radiation cooling takes place at rates of only a few degrees per day. The thin, cold layer did not develop into a major storm, although low-level cloud or fog formation might be expected. As the cold air moved off the coast, it was rapidly warmed by the ocean, but deep clouds did not develop.

Our tentative findings need further confirmation. We are planning to simulate the dynamics associated with longer term, deeper cool layers. There is also a need to couple the dynamics of the model with smoke absorption, to add the effects of water condensation on dynamics, and to study the effects of multiple plumes and how quickly they may merge.

Global-Scale Climate Modeling. During FY 1984, we obtained preliminary results of global-scale climate modeling with the first climate model that interactively coupled smoke absorption and spreading of the smoke by dynamics. These results were obtained by coupling our Lagrangian parcel advection code, GRANTOUR, to the Oregon State University two-level tropospheric general circulation model (OSU GCM). During FY 1985, we refined the smoke transport and removal algorithms and further analyzed the results. In particular, convective mixing of smoke was made consistent with the treatment of moist convection in the GCM. The scavenging mechanism was evaluated and improved. A parameterization for particle coagulation was added which, because of the small scavenging rates assumed for the sub-micron particles, proved to be the dominant removal process for sub-micron particles during the first week following a large smoke injection. This parameterization needs further evaluation, especially since it is a process not now being treated by other modeling groups. The new smoke solar radiation code was vectorized, resulting in a three-fold increase in the model integration speed, which had been significantly slowed when smoke was introduced. With these refinements, a new series of experiments was performed for January, March, and July meteorological conditions, assuming injections of 150 Tg of smoke. (Some of these results were presented in the May 1985 issue of *Energy and Technology Review* of LLNL.) For July, 50 Tg and 450 Tg injections were also performed. Analysis of model results has indicated that, as expected, the sensitivity is greatest for the July injection. Precipitation was identified as a particularly sensitive climate component (see Fig. 13), with significant reductions in land precipitation lasting beyond the period of surface

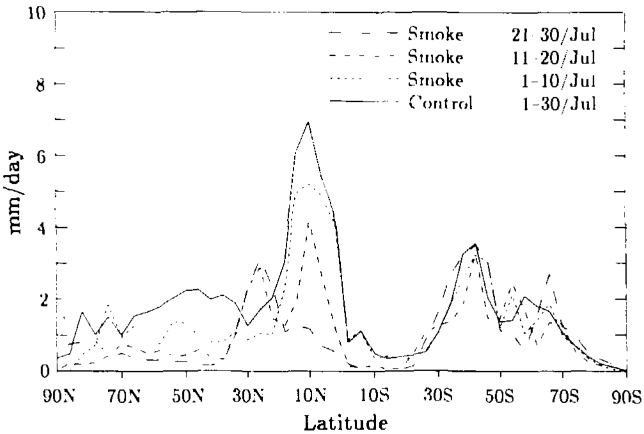


Figure 13. Zonal average daily precipitation rate for ten-day periods following Northern Hemisphere injection of 150 million tonne of smoke.

cooling. This, of course, has important implications for the smoke lifetime in the atmosphere.

In work in association with consultant Robert Cess of the State University of New York at Stony Brook, we used a one-dimensional radiative convective model (RCM), similar to that used by Turco et al. (1983), for detailed study of the climate response and to identify major forcing mechanisms that would also be at work in general circulation models. We found that convective coupling—which normally acts to determine surface and tropospheric temperatures—was unimportant in an atmosphere perturbed by smoke even for modest smoke amounts. Because of this, the model's response could be described as due to either direct surface-troposphere heating or direct surface cooling. These two processes could produce quite unusual time-dependent behavior. For example, the short-term response to a given smoke injection could be one of cooling, while the long-term response could, for some smoke amounts, be one of slight warming.

For non-moving smoke, we also investigated how the climate response would vary as a result of smoke amount, vertical distribution of the smoke, and the initial synoptic conditions that prevail at the time of smoke injection. Figure 14 shows the dependence of temperature response on the absorption optical depth of the smoke (an absorption optical depth of 1 covering the Northern Hemisphere is about equal to 100 million tonnes of smoke). Quite clearly the response is very sensitive to decreasing the smoke amount below values typically suggested. At the present time, we are completing a study of the effects of smoke-laden water clouds (dirty clouds) on the climate response. It appears that such clouds evaporate due to solar absorption, thereby allowing more solar radiation to reach the surface, but providing less infrared (IR) feedback.

As part of the Physics Department's Institutional Research and Development general circulation modeling program, the NCAR nine-level Community Climate Model (CCM) was transferred and adapted to our computer system. As part of the Laboratory's study of the environmental consequences of nuclear war, this model has now been coupled to GRANTOUR and preliminry experiments have been run. Modification to the radiation subroutine to include the IR effects of the smoke particles was done by Curt Covey of the University of Miami during a three-month visit to LLNL. This feature will be important, because the enhanced downward IR radiation from thick smoke patches at early times could moderate surface cooling, and because the enhanced IR emission by the particles could limit lofting of the smoke into the stratosphere. Finally, a delta-Eddington formulation for solar radiation, similar to that adapted to the OSU two-level model, has been prepared for the NCAR CCM (also by Curt Covey), thereby allowing treatment of the effects of scattering by smoke and dust particles. With LLNL support, scientists at NCAR have been developing and testing a boundary layer parameterization that will allow treatment of diurnal effects with the

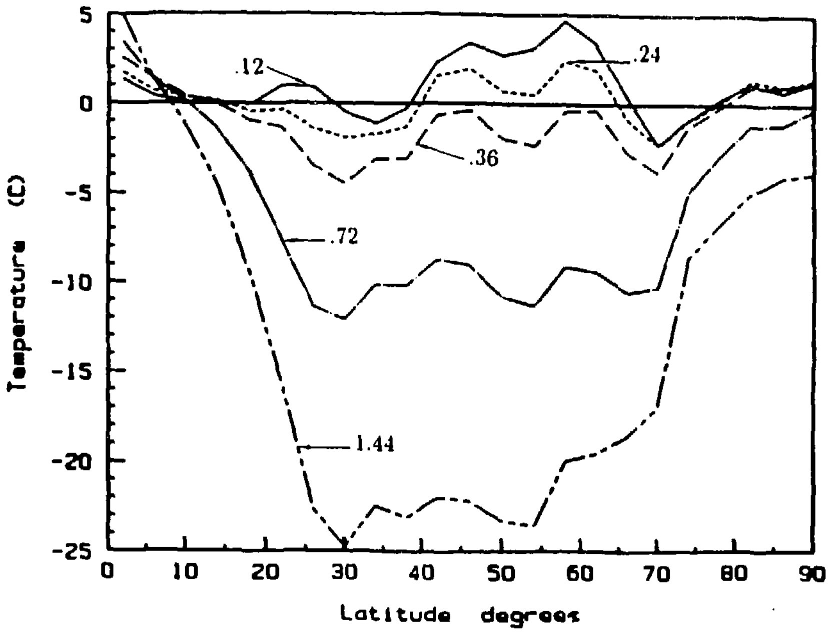


Figure 14. Zonal average temperature change over land as a function of absorption optical depth.

NCAR CCM. Results of preliminary studies indicate that smoke is rapidly (within several days) carried into the stratosphere as a result of heating in the upper-most atmosphere. An initial test run of the model, including the effects of IR absorption and emission by the smoke particles, has also been performed.

Next year, we plan to experiment further with the NCAR CCM on intermediate time scales (1 to 30 days), and with the OSU GCM on extended time scales (1 month to several years). Our preliminary experiments with the NCAR model leave considerable room for improvement. In the present coupled CCM-GRANTOUR model, the number of parcels has been restricted to about 20,000 (i.e., the global atmosphere has been divided into 20,000 equal mass parcels of air). That is too few to represent the distribution of smoke with the same accuracy as the meteorology is treated in the NCAR CCM. Modifications to GRANTOUR are in progress to allow several times more air parcels to be treated. We are now refining the smoke transport and removal mechanisms. So far, IR effects of smoke have been considered only for a specified uniform distribution of smoke. This feature will subsequently be added to the coupled CCM-GRANTOUR model.

Previous modifications to the CCM left it unchanged from the NCAR version in the absence of smoke. The great advantage of this is that the control (no smoke) climate for the model is well known. However, in order to treat the effects of scattering by smoke and of enhanced tropospheric stability on near-surface convection, modifications to the control version of the NCAR CCM are necessary. A new control climate will then have to be developed which, just as for the previous control climate, will differ somewhat from observations. Although development and evaluation of a new control climate will take some time, it is a necessary step in order to treat what are considered important processes. We will then be able to study the effects of a layer of dust shielding smoke from solar radiation, which may inhibit the lofting of the smoke into the stratosphere.

In anticipation that smoke residence times could be several months to more than a year, preparations are being made for extended experiments. These will necessarily involve modeling of the thermodynamic, and possibly dynamic, aspects of the ocean mixed layer. Presently. G-Division has available an ocean mixed layer model that is coupled to the OSU two-level model as part of continuing experiments on the climatic effects of increasing CO_2 concentrations in the atmosphere. However, the OSU GCM specifies but does not simulate the stratosphere. Because experiments with the NCAR model (Malone et al., 1985) indicate that much of the smoke remaining in the atmosphere over long periods would reside in the stratosphere rather than the troposphere, a simulation of the stratosphere is necessary. Thus, either an interactive stratosphere must be added to the OSU GCM or an interactive ocean must be added to the NCAR CCM. We are presently considering how best to meet these requirements.

Biological and Ecological Effects. In June 1984, we sponsored a workshop for the purpose of developing a research agenda to study the biological consequences of "nuclear winter." The workshop goals were to define the biological issues and problems, to outline the existing literature relevant to the problem, and to suggest new, additional research needed to gain knowledge in critical areas. Twenty-seven speakers/attendees discussed the issues over four days. At the end of each session. writing assignments were made for each participant and a chairman was designated for each chapter. We have been working with individual authors to produce a final document (Kercher and Mooney, 1986).

Calculation of the long-term biological and ecological impacts of nuclear war is very difficult. The basic data to properly define initial conditions (damage) do not exist, and the state-of-the-art models needed to simulate the response of the modeled system do not exist. The problem of predicting the biological and ecological effects of the less severe climate changes now thought to be appropriate is far more difficult than prediction of the effects of the severe climate change first suggested by Turco et al. (1983). Still, it seems important to devote resources to study this issue in order to develop the capability to properly assess the ultimate biological and ecological issues.

During FY 1985, we worked on the development of an LLNL program to study the ecological consequences of the potential severe climatic consequences of a nuclear war. For this program, we have:

1. Developed an outline for a national program for an integrated assessment of the effects of "nuclear winter."
2. Suggested an LLNL assessment strategy involving the prediction of impacts at the organism, community, and regional level. At each level, additional research in either experimental or modeling studies (or both) is needed for realistic assessment of impacts. At each level we have identified critical areas for LLNL to make a contribution:
    a. Organism level. We have negotiated a contract with scientists from the University of Wisconsin to conduct experiments on vegetation with simulated climate scenarios using a unique environment-controlled facility (Biotron). These experiments are being performed for a range of plant types and for a range in intensity of temperature and light regimes.
    b. Community level. We have identified an existing LLNL model for forest growth (SILVA) that can be modified to make preliminary assessments of rates of recovery from severe impacts.
    c. Regional level. We have initiated a regional modeling project to study rates of recovery of impacted ecological communities.

Additional LLNL Studies on the Effects of Nuclear War

The recent interest in the potential effects of smoke emissions has led to a resurgence of interest in all potential environmental effects of a nuclear war. Related studies of two potential effects that received earlier attention at LLNL are underway.

Radionuclides. Most of our recent efforts on radionuclides have been inspired by our participation in writing a chapter for the SCOPE-ENUWAR book, ***Environmental Consequences of Nuclear War*** (Pittock et al., 1986). Thus, the work on global fallout doses was extended to take account of the effects of a "nuclear-winter" perturbed atmosphere. This was accomplished by using wind fields predicted by the OSU GCM the GRANTOUR model to carry radionuclide particles and to determine their lifetime in the perturbed atmosphere. Because the perturbed atmosphere is more stable and the hydrologic cycle is suppressed, atmospheric lifetimes are increased and global fallout doses decrease about 15%. Fallout doses were predicted for summer and winter conditions and the results from GRANTOUR were compared to those of the GLODEP2 code, which had been previously calibrated on the fallout doses that occurred during the atmospheric testing in the 1960s.

Local fallout doses are being predicted using the KDFOC2 code. Apparent differences between our code and the traditional approach have been resolved. We are now starting to develop local fallout estimates for the continental U.S. in a study supported by the DNA. Data base development and scenario runs are needed to complete this work.

Atmospheric Chemistry. There is concern about the effects and impacts of chemical emissions from both the explosion and from the fires. Work in this area was also inspired primarily by the invitation to participate in writing a chapter for the SCOPE-ENUWAR document. In the book, our earlier results were summarized, and our emissions estimates were compared to those in the National Research Council (NRC, 1985) report. Apparently a great deal of confusion still exists about emission rates for noxious gases from fires. Back-of-the-envelope calculations indicate that local concentrations of pollutants such as CO could get very high in some areas. Improved calculations are needed and being considered as part of the Labortory's on-going studies of the environmental consequences of nuclear war. Ozone production in the lower atmosphere (smog) does not appear likely on a global scale, although further work is needed. Predictions are very difficult at the present time, because of the uncertain role of heterogeneous chemical reactions between gas-phase products and smoke. Under certain assumptions about these reactions, wide-scale ozone production could occur after the smoke begins to clear. Real progress on these issues will probably occur only after the chemistry of the troposphere is better understood, which may take several years of basic research.

As part of the SCOPE/ENUWAR project, we also have recalculated potential stratospheric ozone depletion, although not yet for the case of a climatically perturbed atmosphere. In our climatically unperturbed atmosphere, the effect of nuclear war on stratospheric ozone has become less over the last decade as yields of weapons have declined. Smoke, its subsequently induced warming and transport in the stratosphere, may, however, cause increased depletion of ozone. Addition of interactive chemistry to global models is needed and may be included in the Environmental Consequences program in the coming year.

Regional Modeling

Research in Progress

The goal of this research is to develop the capability to accurately predict the transport and diffusion of pollutants over complex terrain in the planetary boundary layer. In order to do that, we must be able to accurately model the evolution of the wind, temperature, and turbulence fields, and the pollutant concentration. To meet this objective, we have continued to develop and refine our two- and three-dimensional, time-dependent, non-hydrostatic computer models so that they generate accurate though approximate solutions to the governing primitive equations.

Our modeling effort is unique in that we solve the non-hydrostatic equations of motion via the finite-element method. By using the non-hydrostatic equations, we can simulate a wider range of situations such as non-hydrostatic lee waves or afternoon thermal convection than would be possible with the hydrostatic assumption. With the finite-element method we can also extend the range of situations that we can simulate because it approximates geometrically complex domains accurately and easily. Furthermore, the ease with which differential zoning can be used in this method allows us to use fine zoning only where necessary, such as regions of high gradients either in the boundary geometry or the solution fields.

Currently, we have two related computer models that are used in these studies. The first model, developed with partial support from the Division of Environmental Control Technology of DOE, is directed primarily toward the simulation of the atmospheric dispersion of heavier-than-air gases. This model uses a set of generalized anelastic governing equations that precludes acoustic waves yet permits the large density changes often seen in these cases. This code can also solve the more restrictive Boussinesq equation set as an option. The second model is directed toward simulations of the dispersion of passive pollutants in the planetary boundary layer. These simulations often involve flows that

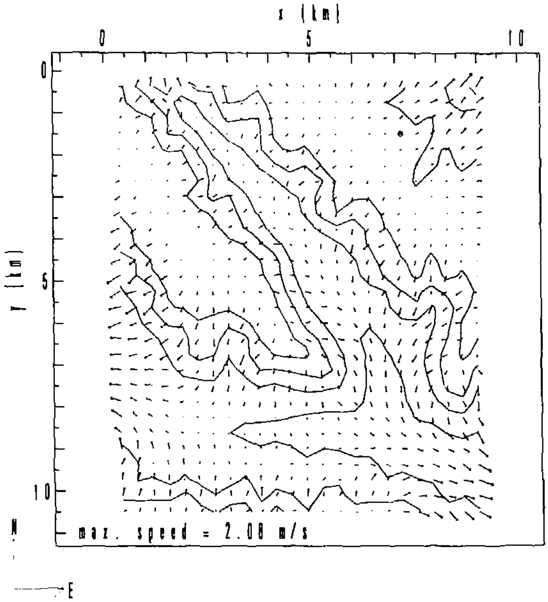


Figure 15. Horizontal velocity vectors at 75 meters above the ground developed by two hours of surface cooling in a neutral atmosphere initially at rest.

interact with complex topography, such as forced flow over hills or katabatic flows due to the cooling or heating of irregular surfaces. This model uses a set of Boussinesq equations and includes the constant rotation Coriolis acceleration.

Because both of these models are subject to continuous development, we have continued our program of model verification to assure that the enhancements do, in fact, increase the models' accuracy and cost-effectiveness. We use various comparisons to measure and evaluate their performance: (1) comparison with analytic solutions (rare), (2) comparison with other numerical results for well-defined problems, (3) comparison with laboratory-scale controlled experiments, and (4) comparison with measurements in the free atmosphere. An example of the last of these is seen in Fig. 15, which shows results from a simulation of drainage flow in Brush Creek, Colorado, the site of recent ASCOT experiments using our planetary boundary layer model.

Program Accomplishments

The most significant accomplishments made during the past year were the major reduction in execution times achieved in both the heavy gas dispersion model and the planetary boundary layer model for large scale simulations. The increased efficiency was achieved by changing from a direct to iterative linear equation solver and developing a new time integration algorithm.

The iterative linear equation solver we adapted to solve the discretized pressure equation was the incomplete Cholesky conjugate gradient method (ICCG) (Kershaw, 1978). Previously, we had used a direct profile solver, which was very efficient if the simulated problem was small enough to be contained completely in the computer memory. However, for all but the simplest three-dimensional simulations this was not possible, and the performance of the solver degraded rapidly as the size of the files kept on disk increased. The use of the ICCG method significantly increases the size of a problem that can be solved in memory, greatly reduces the input/output cost, but sometimes increases in calculations, which are usually less expensive on modern supercomputers.

The next significant improvement was the development of a new, semi-implicit time integration scheme. In most of the simulations we perform, the structure of the flow near the ground is very important. To adequately resolve the flow in this region, thin (typically less than 5 m high) elements are usually required just above the ground. For an explicit code, the use of those thin elements causes significant restrictions on the allowable time-step size (because of stability limits) and, thus, increases the cost of the simulation. Therefore, a less restrictive and more cost-effective time integration algorithm is highly desirable.

Our first step in this direction was to develop of a semi-implicit scheme that was unconditionally stable for the advection-diffusion equation. We then generalized this scheme to the two dimensional Boussinesq equations (Gresho and Chan, 1985). The generalized scheme has no diffusion stability limit, which makes it appropriate to use in combination with a predictive turbulence model in which the diffusion coefficients may vary widely and the stability limits are not generally known at the start of a simulation. And while this new algorithm is only conditionally stable with respect to advection, the stability limit has been observed to be much less restrictive than that of the explicit scheme. In fact, the new semi-implicit time integration that solves the two-dimensional, Boussinesq equations has allowed us to use time steps from 5 to 10 times larger than those previously required by the explicit integration scheme while it retains the same accuracy.

Additionally, as part of our continuing effort to increase types of physical processes that we can simulate, we added a water phase-change submodel to both the heavy gas dispersion model and the planetary boundary layer model (Leone, Rodean, and Chan, 1985). The major assumptions in this submodel are: (1) water exists in only two phases, vapor and condensed, (2) the two phases are in equilibrium, and (3) there is no precipitation. While this submodel does not allow us to simulate all the processes that involve water, it does enable us to simulate the dynamic effects of density gradients caused by the variations in the water vapor distribution. Also, we are able to simulate both the dynamic and thermodynamic effects of condensation and evaporation on the field variables.

To enhance our ability to accurately model actual geographical locations, we have developed a code that allows us to access the extensive ARAC digitized terrain data base. This data base currently contains the topographic data, at a resolution of 65 meters, for the United States and several other countries, and its areal coverage is being continually increased as the data become available. The interface code converts the ARAC data into a form usable by our preprocessor code and thereby enables us to design meshes using the actual topography around any point in the ARAC terrain data base.

Furthermore, we have developed an axisymmetric version of both the generalized anelastic and the Boussinesq equations. These new capabilities will increase the number of phenomena that can be investigated in the less expensive two-dimensional format.

Future Research

The thrust of our efforts in the future will remain basically the same as at present: continued development and application of high-fidelity, numerical techniques directed toward accurate and cost-effective simulations and, ultimately, predictions of pollutant transport. Specifically, we are now adding more sophisticated turbulence submodels to both the planetary boundary layer and the heavy gas models, continue research to extend the capability and cost-effectiveness of the semi-implicit time integration scheme, and continue our model validation program. We will compare results from the planetary boundary layer model against laboratory results for flow around simple three-dimensional hills and against the ASCOT field data from Brush Creek, Colorado. We will also compare the heavy gas code results against both laboratory and field scale experiments such as those conducted by Professor Havens for the Gas Research Institute at the University of Arkansas , the Thorney Island trials (i.e., experiments) by the British Health and Safety Executive, liquid natural gas and propane spill tests by Shell Research, and future field experiments to be conducted by LLNL at the Nevada Test Site Spill Test Facility.

Atmospheric Studies in Complex Terrain (ASCOT)

Research in Progress

The ASCOT program is designed to evaluate pollutant transport and diffusion processes associated with valley flows. It is an integrated program that includes a wide spectrum of analytical and numerical modeling activities and field experimental studies performed by various DOE and National Oceanic and Atmospheric Administration (NOAA) laboratories. Field studies were conducted in The Geysers area in northern California during 1979, 1980, and 1981 and in the Brush Creek valley in western Colorado during 1982 and 1984. The goals of initial experiments were primarily to evaluate the wind, temperature, and turbulence characteristics of the flows, while the later experiments were principally designed to investigate the mass, momentum, and energy fluxes associated with the slope, valley axis, and small tributary flows, as well as the interactions of the valley flows with the larger scale regional flow systems. The modeling studies have ranged from the development of simple analytical models and evaluation against experimental data collected on simple slopes to three-dimensional diagnostic and time-dependent models that have been evaluated against the full data sets generated by these experiments.

The role of LLNL since the inception of the program has been associated with the following: (1) scientific management, (2) numerical modeling, and (3) experimental field studies. The principal management functions during the past year were to plan and conduct a major ASCOT data analysis meeting at mid-year, during which the LLNL management responsibilities were transferred to other laboratories as part of a planned rotation of such tasks.

The modeling effort of the ASCOT program at LLNL was devoted, to a large extent, to the simulation of the tracer release episodes using the three-dimensional transport and diffusion model MATHEW/ADPIC (M/A). The underlying purpose of this model research and development work is to generate with a known degree of confidence a local-to-regional-scale air-quality model that is capable of estimating pollutant concentrations under varying conditions.

In addition to model development, the LLNL numerical modeling effort in the ASCOT program has also included development of a three-dimensional, time-dependent, nonhydrostatic finite-element model. When fully validated against ASCOT field data, this model will provide a cost-effective way to study and understand the dynamics of flow in complex terrain. The results of this model have been compared with the two-dimensional data provided by the Rattlesnake Mountain, Richland, Washington, data set and are currently being validated against the three-dimensional Brush Creek data.

A significant fraction of the LLNL ASCOT resources during the past year were devoted to processing and analyzing of the data generated during the 1984 field experiments in the Brush Creek valley. The data was generated by the LLNL optical anemometers, meteorological towers, a tethersonde, and integrated with similar data acquired by measurement systems fielded by the other program participants. This integration and analysis will broaden our understanding of the characteristics of nocturnal valley flows and enhance our capability to predict the dispersion of pollutants entrained within valley flow systems.

Program Accomplishments

In the modeling area, we realized several major goals. The M/A models were converted from flat terrain applications, where they were originally validated, to the complex terrain and valley flow studies of the ASCOT program. The MATHEW code, which provides the windfield for ADPIC, was modified to accept multiple vertical wind profiles as measured in the experiments. The prescription of the ADPIC diffusivity parameters, especially for the vertical direction, were modified to be able to represent the complex structure of the boundary layer over The Geysers, Anderson Springs, and valley. For better resolution of the pollutant plumes and the corresponding concentration values close to the source of pollutants, a nested grid approach was developed to increase by a factor of 16 the resolution over the rest of the grid.

Considerable effort went into the M/A validation using the extensive meteorological and tracer data of the 1980 Geysers experiment. All four significant drainage flow experiments were simulated with M/A, comprising some 831 data points of time averaged, sequential surface and elevated concentrations. The results indicate some loss of model skill over those validations done in flat terrain. The Geysers experiments were conducted in complex terrain under complex meteorological and difficult experimental conditions, whereas the earlier experiments were conducted in simple terrain and with near neutral stability. Figure 16 shows that, for the Geysers, about 50% of the computed samples agreed within a factor of 5 of the observed, while this factor is about 2 for flat terrain.

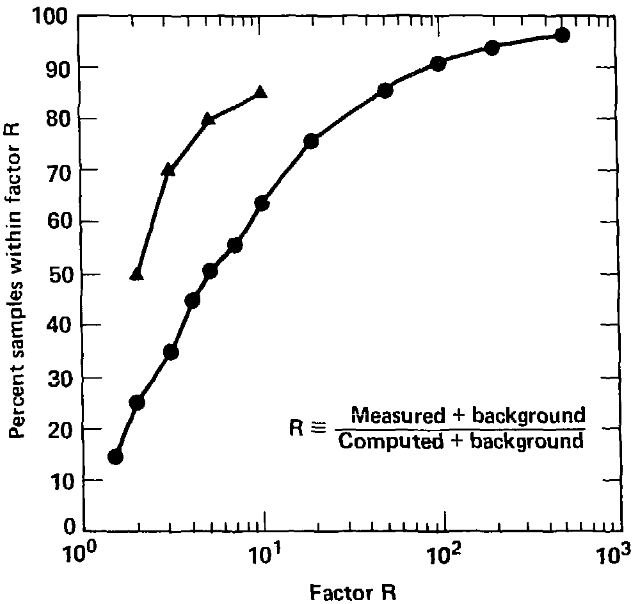


Figure 16. Percentage of computed samples within a factor R of measured concentrations for four tracer experiments in The Geysers (lower curve). The upper curve represents results from the 1972 INEL and the 1974 SRP model evaluation studies.

Part of the LLNL modeling effort consisted of an attempt to determine the trade-off between the degree of complexity of a numerical air-quality model and the quality (density) of the experimental data base used to model tracer scenarios in complex terrain. The model chosen was M/A, because it lends itself to simplification and reduction in skill from a fully three-dimensional K-theory model with terrain to a simple Gaussian continuous point source (cps) model. The extensive 1980 Geysers data set included 8 vertical wind profiles, some 47 surface wind station measurements, and 3 tracer releases that produced about 600 air concentration samples per experiment. Experiment No. 4 was chosen and the wind information in the set was systematically reduced until only the surface wind at the source remained an input measurement. A matrix of computer runs was then made using M/A, with versions of decreasing skill representing the rows of the matrix (A to F) and meteorological input data sets of decreasing quality representing the columns (1 to 5). Table 3 shows the matrix results, in which each matrix element represents the percent of computed samples that were within a factor of 5 of the measured values. It is doubtful that the results of Table 3 can be quantitatively transferred to other locations or other scenarios, but some useful conclusions can be drawn from the trends in the matrix.

A small-scale field study within the Brush Creek valley was conducted this year to confirm prior optical anemometer measurements for evaluating the contribution of tributary flows to the main valley flows. Analysis of the data from the tributary flow experiments revealed unexpectedly large flow variations within the region where the tributary and main valleys merge. Initial estimates reveal that a tributary may contribute up to a few percent of the total valley flow.

Analysis of surface wind measurements in complex terrain reveal values of σ_θ, which are higher by factors of 3–5 over those measured in relatively flat terrain. Median values generally range between 30–40°, on the average, inversely proportional to the wind speed.

Table 3. Sensitivity of model complexity to data base. Anderson, Gunning and Putah Plumes, Experiment of Sept. 19/20, 1980. The elements of the matrix table represent the percent of computed samples of all three plumes that were within a factor of five of measured values. Approximately 600 samples per matrix element.

Decreasing Data Quantity (data base quality) →

Model: Versions of MATHEW/ADPIC ↓ Decreasing Model Complexity	Experiment:	1	2	3	4	5
	Vertical Profile	8	1	1	1	(1) **
	Surface	47	47	25	12	3 ***
A	3-Dimensional, Topography. Gradient Diffusion with K_h, K_z profiles. Winds U,V,W=f(x,y,z), Mass Adjusted.	53	47	43	40	32
B	3-Dimensional, Topography. Gaussian Diffusion, σ_y, σ_z. Winds U,V,W=f(x,y,z), Mass Adjusted.	44	42	39	36	32
C	Sequential Puff, Flat Terrain. Gaussian Diffusion, σ_y, σ_z. Winds U, V = f(x, y, z), W=0, Interpolated.	38	37	36	35	30
* D	Segmented Plume Trajectory (SPT). Gaussian Diffusion, σ_y, σ_z. U, V = Winds at Source, Time Variable.	25	25	25	25	25
* E	Continuous Point Source (CPS). Gaussian Diffusion, σ_y, σ_z. 1 Hour Release. U, V = Winds at Source. Steady.	26	28	28	28	28
* F	Continous Point Source (CPS). Gaussian Diffusion, σ_y, σ_z. Steady Release. U, V = Winds at Source. Steady.	18	18	18	18	18

*These simple Gaussian models use only the wind at the source.
**Estimated power law profile.
***One wind at each of the 3 sources.

Future Research

The first priority will be to evaluate M/A with the 1984 Brush Creek ASCOT experimental data set. Most of the data have been reduced, and tracer transport and diffusion simulations will be conducted for the various release scenarios. This effort is expected to be quite extensive, because, in contrast to the Geysers experiments, the morning transition periods as well as the drainage flow periods were part of the experiment. An important result of this study will be the answer to the question about how well M/A will transfer from the Geysers to Brush Creek without any model tuning.

Improvement of the ADPIC diffusion coefficients is an important ongoing effort. During the Brush Creek experiments, the ASCOT teams collected a large amount of turbulence data, from which diffusion parameters will be derived and tested with the ADPIC model. Of great importance here is the need to provide the model with the capability of handling multiple vertical dispersion layers as were observed in the field. Another question to be addressed is how the canyon walls affect horizontal dispersion. Also, for the first time in the ASCOT program, turbulence data for neutral and unstable conditions will be available to be tested in ADPIC.

Remote sensing wind information from lasers, sodars, and lidars input to M/A is becoming an important step in the evolution of utilization measurements for model evaluations. The amount of lidar data collected in Brush Creek alone could, for the first time, provide windfield input to MATHEW for a significant fraction of its total number of cells. Although space-averaged input, as provided by remote sensing instruments, is desirable for grid models, the best method of using the data has not yet been determined. One approach we intend to pursue is to use only part of the lidar data as input and to try to validate M/A against the rest of the data as a test of MATHEW.

Although diagnostic windfield models like MATHEW have performed well in the ASCOT modeling work, particularly because they can utilize amounts of data, we intend to link our LLNL hydrostatic, dynamic finite-element model (FEM) with ADPIC to study Brush Creek tracer dispersion episodes. This will be a new modeling capability in which the FEM will provide ADPIC with dynamically derived windfields with which ADPIC will then transport and diffuse its marker particles. The differences in the results of tracer simulations between a MATHEW-driven ADPIC and a FEM-driven ADPIC should be great interest for future air quality modeling.

In the next year we plan to proceed with work in three main finite-element areas. The first task is to validate the finite-element planetary boundary layer model against the data collected in the Brush Creek field experiment of September–October 1984. Second, we plan to add a more accurate turbulence submodel to the code. And third, we plan to investigate the possibility of using the wind fields derived by the FEM in the ADPIC dispersion model. If such a linkage can be done effectively, it will add to our capabilities the ability to simulate dispersion from point sources.

We will attempt to derive more refined estimates of mass fluxes associated with tributary and main valley flows by more detailed analysis of the meteorological and tracer data coupled with model calculations. Coordination of the analysis of the perfluorocarbon tracer data will be performed by LLNL with participation from other program scientists. We also plan to participate in the planning and management of a small-scale exploratory experiment in the Brush Creek-Roan Creek valleys during the fall of 1986. This experiment will include merging of flows from several valleys to evaluate pollutant transport and diffusion processes on the 50–100 km scale.

Carbon Dioxide Effects Research Program

Research in Progress

Carbon dioxide effects research at LLNL totaled about $2.1 million in FY1985, of which about 25% is performed by others, mainly universities as contracts, joint projects, and through consulting agreements. Our CO_2 program now conducts research in three of the major theme areas of the DOE Carbon Dioxide Research Program: determination of the direct effects of CO_2 on vegetation, directed by J. Shinn of the LLNL Environmental Sciences Division; projection of climatic effects of increasing concentrations of CO_2 and trace gases; and early detection of the projected climatic effects. The last two areas emphasize atmospheric research and will be covered by this report. Because of this program's wide scope and our participation in advising DOE on research management of the climate and detection elements of the program, our efforts are also closely involved with many other aspects of the nation's CO_2 program.

Program Accomplishments

In studying the potential climatic effects of the increasing CO_2 concentrations, our major goal has been to better understand why apparently similar climate models give different estimates of the potential warming from a doubling of CO_2 concentration. Two major projects are underway: a radiation model and a climate model intercomparison.

First, we are coordinating an intercomparison of radiation codes in climate models, which involves about 50 participants from around the world. We are attempting to determine if the perturbations in radiative fluxes are being calculated accurately. A workshop was held during August 1984 in Frascati, Italy, where the results from the first phase of the model comparison were discussed. This workshop was supported jointly by the U.S. Department of Energy, the World Meteorological Organization (WMO), and the International Radiation Commission of International Association of Meteorology and Atmospheric Physics (IAMAP).

A report of the workshop results was published as a WMO report (Luther and Fouguart, 1984). This widely distributed report has received very favorable comments, affirming the need for this activity, expressing support from the international scientific community, and showing appreciation for the progress made. We are now writing a journal article to summarize the results obtained so far and to describe the future plans for the study. Also, we are writing technical report to be published by DOE in the fall of 1986, which includes descriptions of each of the models used in the comparison, tables of all of the model results, and summary analyses of the results. The second phase of the comparison has also been planned, and information packets were prepared and mailed to over 70 prospective participants. This phase includes comparisons of solar and longwave calculations with and without clouds. The calculations are to be completed by February 1986, and a workshop is scheduled for March 1986 at which the results will be discussed and analyzed.

The second project involves intercomparison of climate models, through cooperative efforts with the State University of New York at Stony Brook, Oregon State University, Atmospheric and Environmental Research Inc., and NCAR. We are comparing the sensitivities of climate models with one, two, and three spatial dimensions to a CO_2 doubling and quadrupling. In these analyses, we are examining how the results of each model depends on the particular representations of the oceans, clouds, radiative perturbations, and other factors. Considerable progress has been made with the OSU/CGM control and doubled carbon dioxide model runs. The model has now been run for 30 model years with a coupled two-level, mixed-layer ocean. The purpose of this long run is to evaluate the equilibrium climate generated by the model with increased CO_2 and to analyze the model's seasonal response to the CO_2 forcing.

The remaining work on the expanded model intercomparison project has been confined mostly to planning and preliminary model experiments to determine how diverse models can be successfully compared. We have initiated joint work with several groups, including The Peoples Republic of China Institute of Atmospheric Physics in Beijing, the British Meteorological Office, and the Canadian Climate Center. We have also agreed on a set of ground rules to be used in the preliminary comparison. This initial study will focus on the changes in sensitivity that result as the number of possible feedback mechanisms is reduced. For example, by using a swamp (zero ocean heat capacity) version of the model and running without clouds, ice feedback, soil moisture feedback, or zenith angle dependence, and then perturbing the models with enhanced CO_2, we will attempt to determine the initial forcing and to isolate some of the causes of model differences arising from processes that cannot be eliminated. Our 2-D climate model will also be included in these studies as a tool to test the possible effects of eliminating and reintroducing various feedbacks.

We have also worked to determine the importance of including the diurnal cycle in the OSU/ LLNL GCM. We have found that the lack of a diurnal cycle can introduce errors as large as 25 W/m^2 in the reflected solar flux. Those errors in the calculated fluxes, in turn, impact the meridional transport and the entire planetary heat balance. Another study related to data acquisition and comparison of the model to observed satellite date demonstrated how a GCM could be used to evaluate different satellite data sets and the effect of different sampling intervals (Cess and Potter, 1986).

A second important question we are looking at is the rate at which the CO_2-induced climate changes should occur and how these projections compare with observed changes over the last century. In cooperation with New York University, we are coupling two-dimensional atmospheric and ocean models to study the climatic effects of the slowly increasing CO_2 concentration (rather than simply study the climatic sensitivity to an instantaneous and prolonged doubling or quadrupling). With these studies we will also be able to look at the potential effects of warming at sea level.

To determine how well model results and our understanding match observed climatic behavior, we are carrying out both analysis and modeling studies. Through analysis of land and ocean temperature data over the last 135 years, we are examining to what extent variations in the average surface temperature over hemispheric and global domains are coherent phenomena and to what extent variations may be artifacts of changing areal representativeness of the data. During FY 1985 we carried out extensive analyses of the Northern Hemisphere land temperature record, focusing particularly on the relative importance of different regions contribute to the changing climate. We obtained from NCAR the marine temperature data base called COADS, reformatted it, and transformed it so that both the air and sea surface temperature gridded monthly anomalies could be used in subsequent calculations. Zonal and hemispheric time series were developed and compared with the work of others. The sensitivity of the Northern Hemisphere average temperature to the presence or absence of individual grid points was examined. The hemispheric average proved surprisingly robust, and many important statistical characteristics remained nearly constant over the last century.

We are also searching the climatic record to determine if volcanic eruptions and other factors may influence the climate. To aid in this search, we are using our climate model to determine the differences in climatic perturbations caused by volcanic eruptions at different latitudes and times of the year. Considerable modeling effort was also devoted to study of the effects of climatically important aerosols, including study of the role of Arctic aerosols (MacCracken, Cess, and Potter, et al., 1986), and of the comparative effects of volcanic aerosol layers at different latitudes and seasons. The Arctic aerosol, in contrast to lower latitude aerosols, was found to warm the Arctic, especially in the springtime.

Preliminary studies over the last several years have indicated that increasing concentrations of methane, nitrous oxide, and chlorocarbons (together called trace gases) can act to augment the CO_2 greenhouse effect. In late 1984, we published a DOE Report of our then-current state of knowledge on each important trace gas and made the first attempt to develop standardized scenarios for past and future emissions and concentrations of key trace gases (Wuebbles et al., 1984). We continually update our analyses of trace gas budgets as more data become available. An updated version of the first report is planned for publication by the WMO.

We have also sought to model the effects trace gases may have had on the troposphere and the stratosphere since the beginning of the industrial age in the mid-1800s (Wuebbles, 1985). Emphasis in this study is on comparison of available measurements and trends in temperature, both surface and stratospheric, with concentrations of various trace gases, particularly ozone. The calculations produced trends that are compare favorably to those measured, but also indicate areas of major uncertainties, particularly in the quality of observed changes in upper stratospheric temperatures. The calculated surface temperature change of 1°C since 1850 is much larger than the approximately 0.5°C measured, suggesting the possible importance of ocean-atmosphere interactions not yet included in model studies. A 20-year temperature lag in the model results would prove consistent with data.

We are also investigating tropospheric-stratospheric interactions and the coupling between temperature and atmospheric chemistry (Wuebbles, Owens, and Hales, 1985; Owens, Hales, and Wuebbles, 1985). Several studies were carried out with Andy Lacis of National Aeronautics and Space Administration-Goddard Institute for Space Studies (NASA-GISS) about effects of stratospheric changes in ozone and water vapor concentrations on tropospheric temperatures. Of particular interest was the finding that, as a result of increasing methane concentrations, the water vapor produced in the stratosphere might produce an additional 30% increase in temperature beyond that produced in the troposphere by methane performance. Knowledge of such changes are necessary for future studies in which additional feedback mechanisms will be included.

In the past year, a number of chemical sensitivity studies were done to examine possible uncertainties that may affect ozone. A study was done in cooperation with Dr. F. S. Rowland of the University of California, Irvine, about the possible importance of a new reaction of H_2O with $ClONO_2$, which may significantly increase the calculated effect on ozone from increasing chlorocarbon concentrations, particularly if methane concentrations continue to increase in the future. A series of chemical sensitivity studies and a Monte Carlo uncertainty analysis were done for the soon-to-be-published WMO-NASA report on the stratosphere (Wuebbles et al., NASA/WMO, 1986). The Monte Carlo results indicate that chemical uncertainties are likely to be more in the direction of producing larger ozone destruction than from typical combined trace gas scenarios.

Several studies done in FY 1985 to establish the importance of key measurements of intermediate lifetime species (e.g., $ClONO_2$, H_2O_2) affected our understanding of atmospheric chemistry (Connell, Crutzen, and MacCracken, 1985; Connell and Wuebbles, 1984; Connell, Wuebbles and Chang, 1985). These studies indicate that measurements of species such as $ClONO_2$, H_2O_2 and HOCl would provide important information about the nature of stratospheric chemistry. We have since been coordinating with various measurement groups to access available satellite data of tract gases for application to future studies of the relationship between theory and observations. We now have some of these data, and we should be getting most of the remaining LIMs and SAMS code data in the near future. The data is important to current studies. Several studies in FY 1985 discussed the importance of determining the long-term trends in trace gas concentrations and temperature in both the troposphere and stratosphere, and what could be learned from such measurements (Wuebbles, Owens, and Halls, 1985; Owens, Hales, and Wuebbles, 1985). For example, trends in upper stratospheric temperature and ozone and trends in high-latitude ozone would tell us a great deal about our understanding of atmospheric processes.

Future Research

Climate-related studies over the next several years will emphasize: (1) comparison and improvement of radiation and climate models, (2) study of how the rate of climate change is controlled by the oceans, (3) the potential increasing role of rising trace gas concentrations on climate, and (4) determination of the extent that climate has been changing and identification of the most important factors. Such a coordinated approach should provide steady reduction of the uncertainties that now limit the confidence placed in model predictions.

Summary of Modeling Capabilities

A wide variety of modeling capabilities have been developed in the course of our many research efforts. This section briefly describes the available models, sub-divided into five categories that describe their primary application.

Species Transport and Diffusion Models

CPS Model

This Gaussian, continuous-point-source (CPS) diffusion and deposition model is used in ARAC applications for initial response calculations. It has two modes of operation: (1) with one set of wind and stability inputs and (2) with up to one year of fifteen-minute or hourly averages. The model incorporates deposition velocity, plume rise, radioactive decay, terrain, and washout. In the multi-line input mode, the user specifies whether the release is routine or accidental. The output consists of concentration and deposition contours for various probabilities that specific contour values will be exceeded.

IPS Model

This Gaussian, instantaneous-point-source (IPS) diffusion and deposition model is used in ARAC applications for initial response and safety analysis calculations. Except for plume rise, its features are similar to those of the CPS model. The values of σ_y are determined from Walton's scale-dependent diffusion equation, while σ_z is calculated from a stability-dependent input parameter, K_z. Results agree reasonably well with output from 2BUFF under conditions of relatively flat terrain, steady state winds, and atmospheric stability.

2BPUFF Model

This two-dimensional, axially symmetric Lagrangian model is used for calculating the anisotropic diffusion of particles or gases in a frame of reference that moves with the center of the cloud of particles or gases (Crawford, 1966; Knox et al., 1971). The diffusion coefficients can be time-dependent. An Eulerian grid at the Earth's surface keeps track of the cloud's position and provides the framework for recording air concentrations during its passage. A conversational version of 2BPUFF has been completed; this will enable the occasional user of the model to prepare reasonable output.

Advection-Diffusion FEM Model

This code solves the advection-diffusion equation (for concentration, for example) in which a fixed velocity field is specified as input data. Either time-dependent or steady solutions are available. As a special case, of course, the transient or steady diffusion equation can also be solved.

Tracer Trajectory Model

This model uses data on of winds and temperature to calculate trajectories on an irregular, continental scale grid. A specified number of parcels, injected at different times, locations, and heights, can be used to represent a tracer injection and can be followed over periods of several days to several weeks. Parcel trajectorics may be followed for (1) countant height above terrain, (2) countant parcel potential temperature, or (3) countant parcel pressure. Dispersal of the tracer by eddy mixing (or diffusion) is not considered.

PATRIC Model

This three-dimensional, particle-in-cell (PIC), sequential puff code for modeling the transport and diffusion of atmospheric pollutants (Lange, 1978) was developed as a simplified and accelerated version of our three-dimensional ADPIC transport and diffusion code. PATRIC has no topography and uses interpolated wind fields that enable the code to model 24 h of real time in about 1 min of computer time—a capability that makes the code suitable for annual air quality assessments. It has been included in the LLNL/ARAC suite of codes available for emergency response and assessment calculations. A modified version of PATRIC that is capable of simulating stratospheric flow for the Northern Hemisphere from AFGWC data has also been developed.

SEAC-PATRIC Model

SEAC-PATRIC is a version of PATRIC modified to provide a capability to model pollutant clouds in the upper air of the Northern Hemisphere and to predict flight-level dose rates. PATRIC was chosen because it can simulate transport and diffusion using three-dimensional wind fields. These wind fields are constructed in the ARAC central facility from AFGWC gridded wind data. SEAC-PATRIC can then provide pollutant air concentrations at chosen regions over the Northern Hemisphere. The code was used to simulate 144 h of the time and space evolution of a stratospheric debris cloud like the Chinese nuclear test of October 1980.

MATHEW/ADPIC Model

A new version of the model, suitable for studying long-range transport and chemistry of several days, is currently being developed. This three-dimensional particle-diffusion model calculates the transport and diffusion of a puff or plume in a time-varying atmospheric boundary layer (Lange, Gudiksen, and Peterson, 1975; Lange, 1978). It is based on the PIC concept, with the hydrodynamic aspect being replaced by a three-dimensional, mass-conservative, time-varying wind field provided by the MATHEW code (Sherman, 1978). We have used this computer model to simulate particulate and gaseous concentrations, the deposition of particles with given size distributions, and rainout (from one or more sources) out to distances of several hundred kilometers. In addition, we have compared ADPIC calculations against measurements for many field-diffusion experiments. The MATHEW/ADPIC models are also used in the ASCOT program (Lange, 1981; Lange and Myrup, 1984). We have used the MATHEW/ADPIC codes extensively in the LLNL-ARAC effort for emergency and assessment response, such as the 1979 TMI incident and the subsequent Presidential Commission investigation. A code validation study for the TMI data has been done (Dickerson, 1980).

GRANTOUR Model

A global atmospheric model that uses prescribed winds to transport species using a Lagrangian sampler parcel approach to calculate advection very accurately. The model can also calculate, if appropriate, scavenging (given precipitation rates), coagulation, dry deposition, mixing between air parcels, and radioactive decay. The model has been used to study the movement and dispersion of smoke and radionuclides in an unperturbed atmosphere (see also OSU/GRANTOUR Model).

Radionuclide Models

CAP Model

The Containment Atmosphere Physics (CAP) model capability simulates reactor containment building scavenging processes. This simulation is based on methods of systems dynamics. It has been developed to be flexible and process oriented; i.e., if new physical processes seemed important, the code allows for their easy insertion into its structure. It should, for example, be feasible and relatively easy to incorporate at least some of the important scavenging processes left out of currently used models. This effort requires both the development of the appropriate cloud physics data base and a simulation that realistically describe the scavenging processes inside a containment building when its equation of state is driven by gaseous releases form a melting core.

MISER Model

The MISER code (Edwards and Harvey, 1983) has been developed to model mini-scale hydrology and groundwater transport of radionuclides from a geologic repository to the biosphere. The potential hazard and dose-to-man may be calculated for a limiting individual using well water of an average individual or population in a river-use system. The code solves a steady state hydrology equation for an arbitrary network of one-dimensional flow-stream tubes. Conservation of water and D'Arcy's laws provide the system of hydrologic equations. A propagator method of solution is employed for nuclides transport. The results of the ORIGEN and BIODOSE codes are used for radioactive decay and river-use system doses. Monte Carlo techniques are applied, where appropriate, to account for measurement and spatial uncertainties. A 500-trial simulation involving 54 stream tubes with 8 parallel paths from a lower aquifer through the repository to the upper aquifer and the biosphere required less than 2.5 min of CRAY-1 computer time.

KDFOC2 Model

A versatile fallout model (Harvey and Serduke, 1979) has been developed to assess complex civil defense and military effects issues. Large technical and scenario uncertainties require a fast, adaptable, time-dependent model to obtain technically defensible fallout results in complex demographic scenarios. The KDFOC2 capability, coupled with other data bases available in G-Division, provides the essential tools to consider tradeoffs between various plans and features in different nuclear scenarios and to estimate the technical uncertainties in the predictions.

GLODEP2 Model

The GLODEP2 computer code (Edwards, Harvey, and Peterson, 1984) provides estimates of the surface deposition of worldwide radioactivity and the gamma-ray dose-to-man from intermediate and long-term fallout. The code is based on empirical models derived primarily from injection-deposition experience gained from the U.S. and the U.S.S.R. nuclear tests in 1958. Under the assumption that a nuclear power facility is destroyed and that its debris behaves in the same manner as the radioactive cloud produced by the nuclear weapon that attacked the facility, predictions are made for the gamma dose from this source of radioactivity. Empirical gamma dose models that account for meteorology, weathering and terrain roughness shielding at specific locations are included. As a comparison study, the gamma dose due to the atmospheric nuclear tests from the period of 1951-1962 has been computed. The computed and measured values from Grove, U.K., and Chiba, Japan, agree to within a few percent.

Atmospheric Chemistry, Radiation, and Microphysics Models

Aerosol Coagulation Model

This model solves the kinetic coagulation equation to describe the evolving size distribution of aerosol particles. The model accounts for the collision of aerosol particles due to Brownian motion, turbulent motion, laminar shear flow, and sedimentation. Dispersion of the aerosol is accounted for by specification of a dilution time constant, which may be determined from observations or calculation. A submodel may be used to calculate the absorption and scattering cross section of the aerosol. The model has been applied as a Lagrangian-parcel model to describe the evolution of the size distribution and optical characteristics of smoke and dust particles after a nuclear war (Porch, Penner, and Gillette, 1985; Penner and Porch, 1986). It is currently being revised to consider several vertical layers to explicitly account for vertical diffusion and aerosol sedimentation.

CUMSCAV Model

This cloud scavenging model is used to estimate the removal of pollutants or radioactivity from the atmosphere because of scavenging by convective clouds. The cloud dynamics and microphysics for this model come from the Rand Corporation Cumulus Dynamics Model (Murray and Koenig, 1972), which is two-dimensional in either axial or rectilinear symmetry and uses a bulk microphysics parameterization. Transport of pollutant material in the cloud's field of motion and a compatible bulk microphysical scavenging parameterization (Molenkamp, 1977) have been incorporated to complete the model. The model has been used not only to calculate scavenging by natural convective clouds but also for estimating self-induced rainout from nuclear weapons at Hiroshima and Nagasaki.

STRATSCAV Model

This model is really a module for the 2BPUFF transport and diffusion model. It calculates the scavenging and deposition of pollutant particles as they move through a region of widespread stratified precipitation. The precipitation is assumed to be horizontally homogeneous so a one-dimensional cloud model gives the vertical distribution of cloud, rain and snow. These hydrometeors then interact with the pollutant particles to scavenge, redistribute, and deposit them (Molenkamp, 1982). A surface-based grid gives the horizontal distribution of the removed pollutant.

RAD1 Solar Radiation Model

This model solves the radiative transfer equation for a cloudless, plane-parallel atmosphere using a successive-scattering iterative procedure. The model includes molecular and Mie scattering, along with absorption by aerosols, ozone, water vapor, carbon dioxide, and oxygen. The solar spectrum between wavelengths of 0.285 and 2.5 μm is divided into 83 discrete spectral intervals, and the vertical column is divided into as many as 500 layers, depending on the optical thickness of the atmosphere. The model computes direct solar flux and the upward and downward diffuse fluxes for each spectral interval at each level, accounting for all orders of scattering.

PHOTO2 Model

This model computes photodissociation rates given the vertical concentration profiles and absorption cross sections of the various chemical constituents in the atmosphere. The solar spectrum from 0.187 to 0.73 μm is divided into 119 spectral intervals, and the radiative transfer equation for a cloudless, plane-parallel atmosphere is solved using a successive scattering iterative procedure. Ozone, molecular oxygen, and nitrogen dioxide are the dominant absorbers in this spectral region, and the Schunann-Rung bands of oxygen (0.187 to 0.205 μm) fall within this region.

Atmospheric Kinetics Model

This model is used for detailed studies of the chemical and photochemical kinetics (no transport) of the troposphere and stratosphere. It used advanced mathematical methods to study the kinetics of a well-mixed cell, including the effects of solar absorption for photodissociation processes. We have used this model for evaluating the sensitivity of reaction mechanisms to deficiencies in our knowledge of reaction rates, quantum yield, reaction ensemble, solar constant, and reactant concentration. The model has also been useful for studying the feasibility of using reduced reaction sets in more complex atmospheric models.

Coupled Transport-Kinetics-Radiation Models

Concentrations of important atmospheric trace constituents are calculated as a function of altitude and latitude, with one- and two-dimensional models that use complex chemical and photochemical processes coupled with transport processes simulated by prescribed mean winds and/or diffusion coefficients (e.g., Wuebbles, 1983 a,b). These models were developed as tools to improve our understanding of the processes important to trace species in the troposphere and stratosphere. The models can be used to study effects of perturbations resulting from the prescribed injection of various pollutants, whether from the surface (e.g., fluorocarbons, N_2O, CO_2) or by aircraft, rocket, or atmospheric nuclear detonation. Model capabilities include diurnal or diurnal-averaged, time-dependent results or a rapidly derived steady state solution. Multiple scattering of radiation is included in computing photodissociation rates. Feedback of changes in temperature and density to adjust chemical reaction rates can also be included. The models include interactive radiation transfer, but do not treat feedback of changes in composition on transport. The current model includes 140 chemical reactions and computes the concentration distribution of 44 species.

LIRAQ Model

The Livermore Regional Air Quality Model (LIRAQ) is an Eulerian (fixed spatial grid) regional air quality model that incorporates mass-consistent advection and diffusion, as well as photochemical kinetics (MacCracken et al., 1978; Duewer, MacCracken, and Walton, 1978; Dickerson, 1978). The model uses topography, meteorology, and pollutant source inventories for the particular region of interest. It then computes the time and spatial variations of the pollutant concentrations at ground level and in the subinversion layer. The model consists of a module (submodel) for each major calculational step, such as pollutant transport, chemical kinetics, and the generation of mass-consistent wind fields from meteorological and topographical data. This modular structure greatly facilitates procedures for revising the model and for adapting it to different regions. For example, the chemical kinetics submodel has been revised and expanded without greatly affecting the transport submodel, and the topography and meteorology of one region can be replaced by those of another. Two versions of the model currently exist. The LIRAQ-1 version is designed to focus on the transport of pollutants, without representing detailed photochemical kinetics. Its explicit calculational technique for physical transport can be used for nonreactive pollutants (such as CO), or it can be coupled to simple, nonstiff reaction sets. The LIRAQ-2 uses a modified Gear package to solve large sets of coupled ordinary differential equations with a high-order implicit method. Thus, it is able to handle very stiff reaction sets. These models were originally verified against station data for four days in the San

Francisco Bay Area (Duewer, MacCracken, and Walton, 1978). They have also been applied in the St. Louis, Missouri, area (Penner, Walton, and Umeda, 1983a). The model chemistry was updated in 1981 (Penner and Walton, 1982) and tested with a revised emission inventory and two new prototype days in the Bay Area (Penner, Walton, and Duker, 1983b).

Multi-layer Air Quality Model

This Eulerian code was developed to describe the long-range transport and chemical interactions of air pollutants. Thus, multi-day simulations are envisioned, in which pollutant concentrations may be stored overnight in an elevated layer and re-incorporated into the mixed-layer the following day. This code uses a split-operator method to solve the three-dimensional transport and chemical kinetics equations for air pollutant concentrations. A highly accurate upstream differencing method with an anti-diffusion correction step has been adopted to describe the transport of pollutants. This method was selected over the conventional finite-element method because it preserves positive species concentrations without the need for an artificial smoothing technique that would add artificial diffusion. The code has been developed for use with an arbitrary number of vertical layers, although only a two-layer version has been implemented to date. In the two-layer version, one layer is used to describe the transport of pollutants below the inversion and one to describe the transport; thus, the model accounts for the deepening of the mixed-layer and mixing of air from above during the afternoon. Pollutant source inventories, topography, and meteorology for the region of interest must be developed as input to the model. In the current version, mass-consistent wind fields are first developed in the MATHEW model and then processed for the layer-average winds needed in the Multi-layer Air Quality Model. The model is being tested now for application in the Monterey and Bay Area air basins.

Hydrodynamics Models

FETISH Model

This code is a general-purpose package that can be used to solve the two-dimensional, steady or time-dependent Stokes, Navier-Stokes, or Boussinesq equations in either Cartesian or axisymmetric coordinate systems. It uses the Galerkin finite-element method in either mixed or penalty form for the spatial discretization with a choice of quadrilateral elements. It uses either the trapezoid rule or backward Euler for the time discretization. The systems of equations are linearized via Newton's method, and the resulting linear systems are solved by means of the frontal method.

Hydrostatic FEM Model

This code solves the two-dimensional, Boussinesq equations of motion, taking advantage of the efficiency (in computational costs) of the hydrostatic assumption. It uses both the Galerkin and least squares finite-element methods for the spatial discretization and a two-step (near trapezoid rule) time-integration scheme. When the hydrostatic assumption is valid, this code is more cost-effective than FETISH. A modified version of this code is being used at Iowa State University.

FEM3 Model

This code solves for the velocity, temperature, pressure, species concentrations, and density in two or three dimensions using either the generalized anelastic equations or the Boussinesq equations. The effect of water condensation and evaporation is included as well as either a constant diffusivity or an algebraic K theory turbulence submodel. The spatial discretization is done via the Galerkin finite-element method using the simple multi-linear velocity, piecewise constant pressure element. The spatially discretized equations are integrated in time via mass lumping and a modified forward Euler scheme.

Laser Isotope Separation Model

Developed in support of the Atomic Vapor Laser Isotope Separation program at LLNL, this model solves the two-dimensional Boussinesq equations in either a Cartesian or axisymmetric coordinate system, using bi-linear velocity, piecewise constant pressure elements in space, and either a forward-backward Euler or semi-implicit scheme in time. While the partial differential equations solved are the same as those in the FETISH model, this newer code, which is a useful blend of finite elements and finite differences, is more cost-effective in most practical cases.

FEM Planetary Boundary Layer Model

This code, derived from FEM3, calculates the spatial and temporal distribution of velocity, pressure, potential temperature, and the mixing ratios of liquid water, water vapor, and an inert tracer in two or three dimensions. With the addition of the constant rotation Coriolis force and a non-linear phase change model to describe the effects of evaporation and condensation, the Boussinesq equations constitute the model equation set. As in FEM3, multi-linear velocity, piecewise constant pressure elements are used in space, while the explicit forward-backward Euler scheme is used to advance the spatially discrete equations in time.

Cloud/Mountain Model

This model was originally designed for the numerical simulation of convective, precipitating storms over complex terrain. It is also capable of simulating stratiform, precipitating orographic storms and both hydrostatic and nonhydrostatic mountain waves. Recently, the model has been modified to simulate the dynamics and microphysics of smoke plumes from intense fires. The model is two-dimensional, time-dependent, Eulerian, nonhydrostatic, and fully compressible. It is based on the three-dimensional cloud model of Klemp and Wilhelmson (1978), but differs from that model in several major ways. It is formulated in terrain following coordinates, it utilizes a Rayleigh sponge to simulate a radiative upper boundary condition, the turbulence parameterization and boundary conditions are different, it includes the complete pressure equation, and no linearization is used to simplify the equations. (For a complete description of the model see Bradley, 1985).

CSU Mesoscale Model

We are using the Colorado State University (CSU) Mesoscale Model developed by Pielke and his students to simulate a variety of terrain and surface forced mesoscale flows. This model is a hydrostatic, incompressible, primitive equation model; it includes topography and a detailed boundary layer parameterization. The flows are usually driven by surface heating, which is calculated by balancing the surface energy budget at each grid point. Atmospheric heating by absorption and emission of long and short wave radiation is also included. The model is three dimensional, but it can be run in a two-dimensional, rectilinear mode. For our applications, the CSU Mesoscale Model has been enhanced by allowing clouds and fog to form in saturated regions and by greatly improving the long wave radiation parameterization.

Global Climate Models

Statistical-Dynamical Climate Model

The Livermore Statistical Dynamic Climate Model (LSDM), previously referred to as ZAM2, is a two-dimensional, Eulerian thermodynamic model of the Earth's atmosphere-surface-ocean system in the meridional plane (MacCracken et al., 1981). The model considers a moist atmosphere and includes such effects as solar and infrared radiation, variable cloudiness, precipitation, surface interactions, the variable extent of snow cover and sea ice, and mountains. The seasonal version of the model includes a well-mixed layer and prescribed meridional heat fluxes in the ocean layer. The model has recently been used to test the response to increased atmospheric CO_2, Arctic soot, volcanic aerosol injections, and other perturbations.

Oregon State University/LLNL General Circulation Model

As a part of the ongoing model intercomparison project, a version of the OSU GCM has been customized at LLNL in order to provide a new tool for climate assessments. Consultant Prof. Robert D. Cess improved the solar radiation scheme in the model in order to test the climatic effects of massive injections of smoke and dust resulting from a nuclear war (Cess, Ghan, and Gates, 1985). Through cooperation with the staff at OSU, the model was used one of the first systematic intercomparisons (Potter and Gates, 1984), and it is being constantly modified as one of the key participants of an expanded intercomparison project that will include GCMs from numerous national and international institutions.

Oregon State University/GRANTOUR General Circulation Model

The GRANTOUR species transport model and the OSU/LLNL general circulation model have been interactively coupled so that the species concentrations in the GRANTOUR model may perturb the radiative calculation in the OSU/LLNL GCM and so that the winds and precipitation in the *OSU/LLNL GCM* control the transport and scavenging of species in GRANTOUR. This model has been used extensively to study the potential climatic effects of post-nuclear war smoke injections.

LLNL/Community Climate Model

A version of the NCAR general circulation model (CCM0B) has been transferred to the LLNL computer system and its speed increased by about a factor of two by development of improved memory management routines. Various parameterizations are being improved and added so that aerosols can be treated by the radiative routines. Coupling to the *GRANTOUR* model is underway.

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Appendix A: Organization and Budget

Cognizant Associate Directors
J. H. Nuckolls, Physics
M. M. May, At Large
M. L. Mendelsohn, Biomedical and Environmental Research
G. H. Miller, Defense Programs
K. Street, Energy Resources

Division Leader
J. B. Knox

Deputy Division Leader
M. C. MacCracken

Associate Division Leaders
M. H. Dickerson
P. M. Gresho
F. M. Luther

Program Manager
F. L. Worden

Division Secretary
C. L. Myers

G-Division Scientific Staff

Name	Discipline	Degree	School
Michael M. Bradley	Atmospheric sciences	Ph.D.	U. Illinois
Stevens T. Chan	Mechanical engineering	Ph.D.	U. Calif., Davis
Peter S. Connell	Chemistry	Ph.D.	U. Michigan
Marvin H. Dickerson	Meteorology	Ph.D.	Florida State U.
Leslie L. Edwards	Mathematics	M.A.	U. Oregon
James S. Ellis	Meteorology	Ph.D.	Colorado State U.
Hugh W. Ellsaesser	Meteorology	Ph.D.	U. Chicago
Kevin T. Foster	Atmospheric sciences	M.S.	U. Calif., Davis
Steven J. Ghan	Meteorology	M.S.	M.I.T.
George D. Greenly, Jr.	Meteorology	M.S.	U. Oklahoma
Keith E. Grant	Applied science	Ph.D.	U. Calif., Davis/Livermore
Philip M. Gresho	Chemical engineering	Ph.D.	U. Illinois
Stanley L. Grotch	Chemical engineering	Ph.D.	M.I.T.
Paul H. Gudiksen	Chemistry	Ph.D.	U. Washington
Ted F. Harvey	Physics	Ph.D.	U. Calif., Davis
Joseph B. Knox	Meteorology	Ph.D.	U. Calif., Los Angeles
Kenneth C. Lamson	Health physics	M.S.	U. Pittsburgh
Rolf Lange	Atmospheric sciences	Ph.D.	U. Calif., Davis
Robert L. Lee	Mechanical engineering	Ph.D.	U. Calif., San Diego
John M. Leone, Jr.	Meteorology	Ph.D.	Iowa State U.
Frederick M. Luther	Applied science	Ph.D.	U. Calif., Davis/Livermore
Michael C. MacCracken	Applied science	Ph.D.	U. Calif., Davis/Livermore
Connee S. Mitchell	Meteorology	M.S.	Oregon State U.
Charles R. Molenkamp	Meteorology	Ph.D.	U. Arizona
Joyce E. Penner	Applied mathematics	Ph.D.	Harvard U.
Kendall R. Peterson	Meteorology	M.S.	U. Chicago
William M. Porch	Geophysics	Ph.D.	U. Washington
Gerald L. Potter	Geography	Ph.D.	U. Calif., Los Angeles
Daniel J. Rodriguez	Meteorology	M.S.	Calif. State U., San Jose
Leonard C. Rosen	Physics	Ph.D.	Columbia Univ.
Thomas J. Sullivan	Meteorology	Ph.D.	U. Calif., Davis
Karl E. Taylor	Physics	Ph.D.	Yale U.
John J. Walton	Physics	Ph.D.	U. Kansas
Roger L. Weichel	Meteorology	M.S.	U. Utah
Donald J. Wuebbles	Atmospheric sciences	Ph.D.	U. Calif., Davis

G-Division Supporting Staff

Name	Position
Nancy A. Badal	Secretary
Pamela M. Drumtra	Secretary
Sandra J. Eyre	Secretary
Carol L. Myers	Division Secretary
Lonnette L. Robinson	Secretary
Doris G. Swan	Secretary
Charles R. Veith	ARAC Facilities Coordinator
Floy L. Worden	Program Manager

Affiliated Staff

Name	Affiliation	Discipline	Degree	School
Ronald L. Baskett	6	Atmospheric sciences	M.S.	U. Calif., Davis
Richard D. Belles	1	Applied science	M.S.	U. Calif., Davis
Diane F. Bonner	1	Mathematics	B.S.	State U. of N.Y., Albany
Sharon C. Braley	1	General education		Chabot College
DeeAnn Davi	6	Mathematics	B.A.	Westmont College
Len R. Edwards	6	Math/science	B.S.	Rollins College
K. Patrick Ellis	3	Safety, public relations		
Donald A. Garka	2	Electronics engineering	B.S.	Devry Inst. Tech.
Leonard C. Haselman, Jr.	5	Physics	B.S.	Seattle U.
Patricia Kale	6	Electronics engineering	B.S.	U. Calif., Berkeley
Sang-Wook Kang	4	Aerospace Science	Ph.D.	Rensselaer Polytech Inst.
Leonard A. Lawson	1	Mathematics	A.B.	Calif. State. U., Chico
Ambrosio R. Licuanan	1	Computer science	A.A.	Ohlone College
Ida S. Lozares	1	Mathematics	B.S.	Calif. State U., Hayward
Gloria Martin	6	Computer science		Chabot College
Mary A. Mansigh	1	Math/chemistry	B.S.	U. Miami
Michael Mc Neill	1	Computer science	B.S.	Georgia Tech.
John Nasstrom	6	Atmospheric sciences	M.S.	U. Calif., Davis
Charles O'Connor	1	Computer science	M.S.	Calif. State U., Hayward
Thomas A. Reitter	4	Mechanical Engineering	M.S.	U. Calif., Davis
Raymond L. Tarp	1	Mathematics	B.A.	Calif. State U., San Jose
Sandra Taylor	1	Computer science	B.S.	Iowa State U.
Hoyt Walker	1	Computer science	M.S.	U. Calif., Davis
Patrick P. Weidhaas	1	Mathematics	M.A.	U. Calif., Berkeley
Jon Welch	2	Electronic technology		

1. *Computations* Department (LLNL)
2. Electronic Engineering Department (LLNL)
3. Hazards Control (LLNL)
4. Mechanical Engineering Department (LLNL)
5. B-Division (LLNL)
6. EG&G

Visiting Faculty

Name	Discipline	School
Arthur A. Broyles	general physics	University of Florida
James Ipser	theoretical astro-physics	University of Florida
Robert L. Sani	finite-element methods and applications	U. Colorado
Charles S. Shapiro	nuclear physics, radiation effects	Calif State U., San Francisco

Consultants

Name	Discipline	Company/School
James F. Barbieri	data management systems	private consultant
Alfred K. Blackadar	micrometeorology	Pennsylvania State U.
Robert D. Cess	atmospheric sciences climate modeling	State U. of New York, Stony Brook
Curt Covey	climate modeling	U. of Miami
Robert G. Ellingson	atmospheric radiation transfer	U. of Maryland
John Hallett	ice crystal scavenging	U. of Nevada, Desert Research Institute
Joseph B. Klemp	meteorology, computer science	National Center for Atmospheric Research
Stephen Krueger	turbulence modeling	U. of California, Los Angeles
Richard C. Orphan	resource management	private consultant
William R. Pendergrass	air pollution meteorology	NOAA/Atmospheric Turbulence and Diffusion Laboratory
Robert L. Sani	numerical methods hydrodynamics	U. of Colorado
Charles S. Shapiro	radionuclide dose assessments	California State U., San Francisco
David Simonette	urban fuel loading	University of California, Santa Barbara
Brian D. Templeman	digital mage processing and analysis	NOAA/Atmospheric Turbulence and Diffusion Laboratory
Ronald D. Tilden	creativity enhancement	Tilden and Associates
Wei-Chyung Wang	chemistry, radiation transfer, and stratospheric chemistry	Atmospheric and Environmental Research
Gene L. Wooldridge	micrometeorology	Utah State U.
Morton G. Wurtele	meteorology	U. of California, Los Angeles

G-Division Members Pursuing Academic Degrees

Name	Discipline	Degree	School
Steven J. Ghan	atmospheric sciences	Ph.D.	MIT
George D. Greenly	atmospheric sciences	Ph.D.	Univ. of Calif., Davis
Daniel J. Rodriguez	atmospheric sciences	Ph.D.	Univ. of Calif., Davis
Floy Worden	business administration/ information systems	B.A.	Calif. State Univ., Hayward

G-Division Student Guest

Name	Discipline	School
James Rowley	computational physics	Univ. of Calif., Department of Applied Science, Davis/Livermore

G-Division Budget by Sponsor(K$)

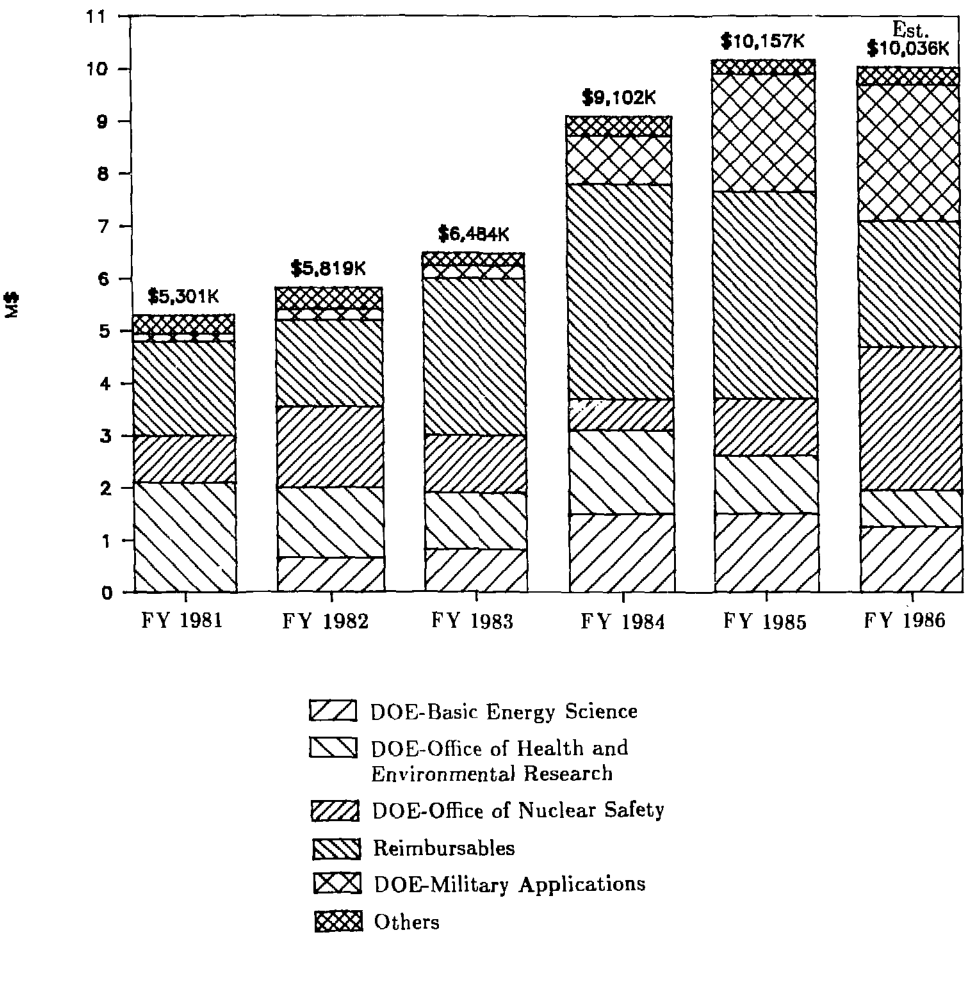

Figure A1. G-Division budget with sponsoring agencies for FY 1981–86.

Appendix B: G-Division Publications—FY 1984–1986

Journal Articles

Cess, R. D., and G. L. Potter (1984), "A Commentary on the Recent CO_2-Climate Controversy," *Climatic Change*, **6**, 365–376.

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Appendix C: Acronyms

Acronym	Meaning
ADPIC	Atmospheric-Diffusion Particle-in-Cell
AEROS	ARAC Emergency Response Operating System
AFGWC	Air Force Global Weather Central
ARAC	Atmospheric Release Advisory Capability
ARG	Accident Response Group
ASCOT	Atmospheric Studies in Complex Terrain
CAP	Containment Atmosphere Physics
CCM	Community Climate Model
COADS	Marine Temperature Data Base
CPS	Continuous Point Source
CSU	Colorado State University
DNA	Defense Nuclear Agency
DOD	Department of Defense
DOE	Department of Energy
DRI	Desert Research Institute
ENEA	Ente Nazionale Energie Alternative (Italian)
ENUWAR	Environmental Consequences of Nuclear War
EOC	Emergency Operations Center
FAA	Federal Aviation Administration
FEM	Finite-Element Modeling
FY	Fiscal Year
GCM	General Circulation Model
G-Division	Atmospheric and Geophysical Sciences Division
GISS	Goddard Institute for Space Studies
GRANTOUR	Lagrangian Parcel Advection Code
IAMAP	International Association of Meteorology and Atmospheric Physics
ICCG	Incomplete Cholesky Conjugate Gradient
ICSU	International Council of Scientific Unions
IPS	Instantaneous Point Source
IR	Infrared
IRF	Incident Response Force
JNACC	Joint Nuclear Accident Coordinating Center
LIMS	Limb Infrared Monitor of the Stratosphere
LIRAQ	Livermore Regional Photochemical Air Quality Model
LLNL	Lawrence Livermore National Laboratory
LSDM	Livermore Statistically Dynamic Climate Model
LSP	Lagrangian Sampling Parcel
M/A	MATHEW/ADPIC
MATHEW	Regional Diagnostic Flow Model
NASA	National Aeronautics and Space Association
NATO	North Atlantic Treaty Organization
NCAR	National Center for Atmospheric Research
NEST	Nuclear Emergency Search Team
NMCC	National Military Command Center
NOAA	National Oceanic and Atmospheric Administration
NWS	National Weather Service
OSU	Oregon State University
PIC	Particle-in-Cell
RAP	Radiological Assistance Protection
RCM	Radiative Convective Model
SAMS	Stratospheric and Mesopheric Sounder
SCOPE	Scientific Committee on Problems in the Environment
TMI	Three Mile Island
USGS	U.S. Geological Survey
WMO	World Meteorological Organization
WP	Warsaw Pact
ZAM	Zonally Averaged (Climate) Model

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