Physics Department
Lawrence Livermore National Laboratory

Atmospheric and Geophysical Sciences Division

Program Report FY 1987

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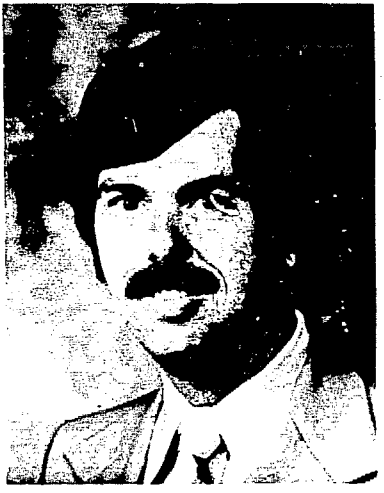

Dedication

Frederick M. Luther
1943–1986

On September 13, 1986, our colleague and friend Fred Luther died of complications arising from his two-year battle with cancer. Fred brought a special mix of scientific insight and personal warmth to his endeavors, always seeking to learn from and build upon the positive aspects of people's talents. His approach allowed him to forge seemingly disparate views into an agreed-upon approach for explaining findings and planning further research. Most recently, he had been instrumental in involving more than 60 researchers from around the world in the Intercomparison of Radiative Codes in Climate Models (ICRCCM), an effort in which all of the investigators must expose their codes to a series of tests that could easily indicate substantial shortcomings in the codes. Fred, however, was able to provide the assurance that everyone could safely take this risk, doing so by focusing attention on the many insights that could be gained and the benefits that all could expect as a consequence of further model improvement.

Fred joined the Atmospheric and Geophysical Sciences Division of Lawrence Livermore National Laboratory in 1972, becoming associate division leader in 1979. During his 14 years with the Division, Fred's interests spanned study of a wide variety of factors that could perturb atmospheric radiation, chemistry, and climate. These included studies of effects from the emissions of nitrogen oxides, chlorofluorocarbons, carbon dioxide, and other human-affected trace gases, evaluations of the injection of volcanic aerosols, and studies of smoke from fires following a nuclear war. This wide range of interests led to his participation in a number of advisory roles, including particularly his service to the Department of Energy's (DOE's) Carbon Dioxide Research Division, for which he served, beginning in 1982, as one of the two area managers for the climate and detection elements. A major achievement on the DOE's behalf was Fred's role as coeditor and coauthor of the two recent state-of-the-art reports on projecting and detecting carbon-dioxide-induced climate change, for which he received a DOE letter of commendation.

Fred's interest in bringing together divergent aspects of problems introduced him to a large number of fellow scientists, with whom he made a wide set of good friends. To these and other friends, in his church and in his many activities, and with his family, he was always open and

affirming, building on the positive, promoting the professional growth of his colleagues, and offering insightful guidance and suggestions humbly. Although Fred had been suffering from lymphoma for two years, he was hopeful that a sequence of treatments could prolong his life for several more years. The treatments did, however, carry him long enough so he could come to an inner peace and, through his life, to have very positively influenced those of us fortunate enough to have been his friends. Fred's presence—his intellect and curiosity, his warmth and compassion, his friendship—are dearly missed.

In recognition of

Joseph B. Knox
Retired December 15, 1987

Joseph B. Knox, G-Division leader, retired December 15, 1987 after a more than thirty-year career with the University of California. Joe received his Ph.D. from the Department of Meteorology, University of California, Los Angeles, in 1955, and then taught for three years in the department before joining the then Lawrence Radiation Laboratory. Joe began his career at the Laboratory developing technical capabilities to simulate the cratering and to evaluate the potential dispersion of radionuclides as a result of the proposed peaceful use of nuclear explosives in construction projects. Building on the experience gained from these studies, his efforts led to development of other projects concerned with the atmospheric dispersal of pollutants. Most prominent was the Atmospheric Release Advisory Capability, which has provided important real-time support to national response agencies during atmospheric releases of radionuclides, including the Three Mile Island (TMI) and Chernobyl events.

As scientific and societal interest in atmospheric and environmental science issues increased, Joe created and assumed leadership of the Atmospheric and Geophysical Sciences Division in 1974, which brought together the Lawrence Livermore Laboratory's atmospheric research on local, regional, and global scales. Under his guidance, this program grew from about ten to nearly eighty scientific and support personnel, with responsibility for almost forty different projects. During these years, the strength and breadth of the program has expanded to include study of space scales from kilometers to global and time scales from hours to years.

Joe has not become inactive. He will continue to be involved with the Division's programs and with Physics Department management (he remains Assistant to the Associate Director for Physics), especially in providing guidance and input to developing future research directions and activities.

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Program Report for FY 1987
Atmospheric and Geophysical Sciences Division of the Physics Department

Abstract

In 1988 the Atmospheric and Geophysical Sciences Division began its 15th year as a division. As the Division has grown over the years, its modeling capabilities have expanded to include a broad range of time and space scales ranging from hours to years, and from kilometers to global, respectively. For this report, we have chosen to show a subset of results from several projects to illustrate the breadth, depth, and diversity of the modeling activities that are a major part of the Division's research, development, and application efforts. In addition, the recent reorganization of the Division, including the merger of another group with the Division, is described, and the budget, personnel, models, and publications are reviewed.

Introduction

The goal of the Atmospheric and Geophysical Sciences Division (G-Division) of the Physics Department at Lawrence Livermore National Laboratory (LLNL) is to contribute to advancing and improving the understanding and resolution of nationally and internationally significant atmospheric and geophysical science issues by developing, applying, and interpreting results from carefully formulated and verified numerical models of the atmosphere–geosphere system. In pursuit of this goal, we combine a highly experienced and diversified professional staff (often involving collaborative efforts with university scientists), a broad range of atmospheric models covering scales from microphysical to global, and participation in field programs and exercises to aid in model verification. Appendix A provides a listing of staff members and Appendix B provides a listing of collaborative activities. A listing of acronyms and abbreviations is included in Appendix H.

G-Division's activities range from research-oriented efforts involving the development of new, more comprehensive process models of local- to global-scale domains, to real-time application of models as part of the Atmospheric Release Advisory Capability (ARAC), which is the designated national response center in the event of potential or actual releases of radionuclides to the environment. Currently, about three-fifths of the support for our research comes from the various parts of the Department of Energy (DOE); the other two-fifths comes from the Department of Defense (DOD), the National Aeronautics and Space Administration (NASA), the Environmental Protection Agency (EPA), the Nuclear Regulatory Commission (NRC), and other agencies and industrial concerns (see Table 1). We actively participate in workshops, meetings, and programs at the national and international level, report on our studies in articles in popular and professional publications, and invite others to present seminars that are of interest to G-Division. (See Appendix C for a list of special outside activities by our staff members and Appendix G for a list of invited speakers for the Division.)

To enhance LLNL's studies on the atmospheric consequences of releases of heavier-than-air gases and toxics, the Laboratory has merged the Liquefied Gaseous Fuels Program (J-Group) with G-Division (responsibility for field studies at the Nevada Test Site remains, however, under the

Table 1. FY 1988 G-Division Budget by Sponsor.

Sponsor Organization	Funding[a] (thousands of dollars)	Percentage
DOE/ER (OHER & BES)	$2,279	20.4
DOE/EH	1,500	13.5
DOE/NR	568	5.1
DOE/DP	1,518	13.6
DOE/FE	160	1.4
Other DOE	383	3.4
DOD	3,015	27.1
NASA	319	2.9
EPA	242	2.2
Nongovernment Organizations	899	8.1
LLNL Institutional R&D Program	200	1.8
LLNL Physics Department WSR	60	0.5
TOTAL	$11,143	100.0

[a]Excludes DOE equipment funding (except DOE/NR) and GPP funding.

Nuclear Test Program). Consolidation of this scientific research with G-Division is permitting us to accelerate our efforts to extend ARAC to treat accidental releases of toxics and heavier-than-air gases, both of which pose serious potential public health threats as the result of accidents involving the storage or transport of such materials on trains, highways, and in harbor areas. In addition, G-Division's modeling and microphysics expertise can be used to help expand heavy-gas modeling capabilities, particularly as they relate to the complex physical characteristics of gases such as UF_6. Closer coordination with the Mesoscale and Fluid Dynamics Group will also be beneficial.

In our research, models play an essential role in seeking to improve understanding of the atmosphere-geosphere system. They:

- Provide a basis for investigating and understanding causes, feedbacks, and responses and for testing hypotheses about how this system functions.
- Are an essential tool in the design of experimental programs and provide the framework within which to interpret and understand observations.
- Can assist in determining the optimal locations for observations to be taken and in developing an observational strategy for investigating issues of importance.
- Can be used to estimate the accuracy required of instruments and their potential value for measuring variables of interest.
- Provide the basis for generalizing localized results and for projecting future conditions.

G-Division maintains a suite of atmospheric models capable of simulating the complex set of dynamic, physical, and chemical interactions that occur upon release or injection of energy-related species into the environment. These models have been and continue to be applied to problems of national and international importance. Table 2 summarizes the set of core modeling capabilities now available in the Division; these capabilities provide the basis for the research conducted by

Table 2. Core Modeling Capabilities.

Transport, Diffusion, Deposition, and Hydrodynamic Models
3-D models of local- to regional- to global-scale dispersion and deposition of radionuclides
2-D and 3-D global fallout models to study nuclear war, power plant accidents, etc.
2-D and 3-D cloud scavenging models
2-D and 3-D heavy-gas dispersion models including phase change and complex terrain
1-D (quasi-3-D) model for heavy-gas dispersion in flat terrain
2-D and 3-D general viscous, incompressible flow and thermal convection models
2-D and 3-D heavy gas dispersion models
2-D and 3-D nonhydrostatic planetary-boundary-layer models based on finite-element methods
Atmospheric Chemistry and Microphysics
3-D regional photochemical-transport model
1-D and 2-D global chemical-transport models, with radiation feedback
2-D and 3-D global tracer models
3-D tropospheric nitric acid formation and deposition model (other chemistry is being added)
Detailed microphysics model of aerosol and warm rain processes
Climate
3-D general circulation model of global atmosphere
3-D general circulation model of troposphere
3-D 2-layer dynamic model of the global ocean
1-D and 2-D simplified climate models of the atmosphere and oceans
1-D multiwavelength atmospheric radiation model

various thematic groups. Appendix D provides a short description of models being used in the Division, with points of contact listed as references for further information.

Division Organization: Thematic Roles, Capabilities and Accomplishments, and Key Issues

The Atmospheric and Geophysical Sciences Division (G-Division) is administratively part of the Physics Department at LLNL, but is involved in research and application studies for and with many other parts of the Laboratory and other governmental agencies. To meet these broad programmatic efforts, the Division is organized into seven thematic groups (see Fig. 1). Summarized below are the roles, capabilities and accomplishments, and key issues for each group, followed by a more detailed example of each thematic group's focus.

Atmospheric Release Advisory Capability (ARAC) Group

Role

The ARAC group is responsible to the DOE, the DOD, and other national agencies for developing and providing real-time assessments of the atmospheric transport, dispersion, and deposition of radionuclides in the event of potential or accidental releases of radionuclides into the atmosphere.

Capabilities and Accomplishments

- Currently serves about 50 DOE and DOD sites.
- Timely responses to more than 175 exercises and all major accidents, including Three Mile Island, Titan II missile, Soviet satellite reentry, and Chernobyl.

Key Issues

- Expansion to include Naval Reactor and remaining DOE sites within three years.
- Growth to 24-hr status.
- Meteorological prediction instead of assumption of persistence.
- Extension to the release of classes of nonradiological toxics.
- International connections and technology transfer.

Focus: ARAC is responsible to the DOE, the DOD, and other national governmental agencies for providing real-time assessments of the transport, dispersion, and deposition of radionuclides in the event of potential or accidental releases of radionuclides into the atmosphere. In addition to the DOE and the DOD, ARAC serves as the major assessment capability for the NRC, the EPA, and the Federal Aviation Administration (FAA) when radioactive material has been released into the atmosphere.

The major focus of this group is to provide an emergency planning, response, and assessment service for the various government agencies it serves. A considerable amount of time is spent each year supporting emergency response exercises conducted by the individual sites and various Federal agencies. Currently the sites consist of approximately 50 DOE facilities and military bases that are connected directly to the ARAC center via modems and computers. This means that a large part of ARAC's effort is spent dealing with the various individual client needs and requirements. At this time the center is staffed 40 hr/wk for an immediate response, and the off-hours are covered by a callout of available staff. The number of staff members is 24. Their experience encompasses meteorology, health physics, computer science, engineering, and computer utilization/support. Within two years we expect that growth in the ARAC service/support will permit an increase in staff and provide an immediate response for 24 hr/day.

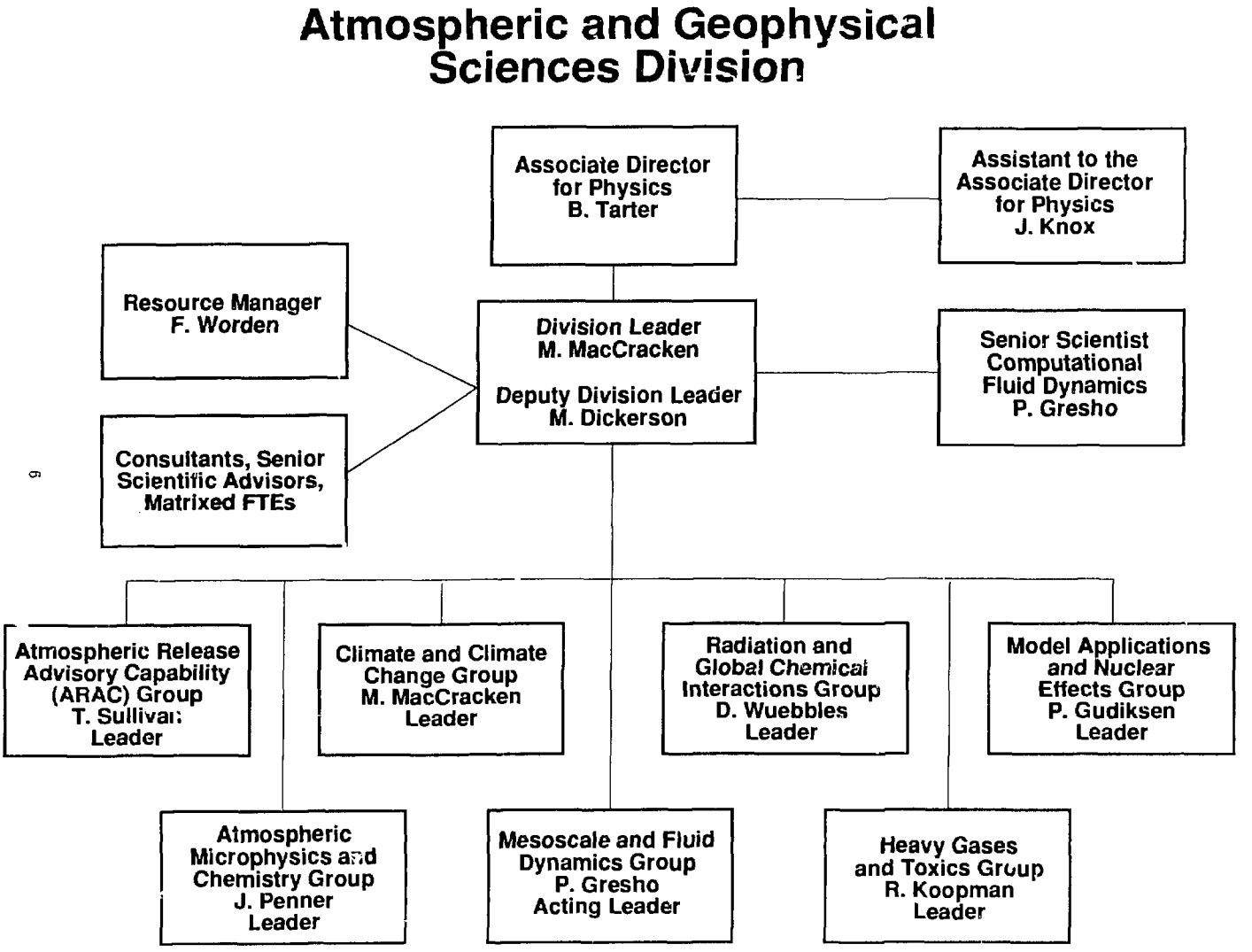

Figure 1. Organizational chart showing the seven thematic groups of G-Division.

The ARAC center is connected to Air Force Global Weather Central (AFGWC) in order to have on-demand access to near real-time meteorological data from virtually every place in the world that reports measurements of wind speed/direction, temperature, pressure, etc. For particular locations in the U.S., these data are automatically transmitted every hour to the ARAC computers, where they are stored and are readily accessible if needed. As previously stated, about 50 DOE and DOD facilities are connected directly to the ARAC center with computers, which transmit meteorological data to the center and receive assessment products from the center.

For locations not initially specified as probable accident sites (e.g., Chernobyl), site-specific databases can be rapidly developed and used. For example, the terrain data for the continental U.S. is on-line and accessible in about four minutes, with a horizontal resolution of 0.5 km. These data can be used directly in the assessment models, and they can be colored and shaded to show topographical details such as mountains and valleys. Assessment models on-line in the center are capable of addressing a wide range of accidents, varying from nuclear power plants and atmospheric tests (e.g., Chinese) to nuclear weapons accidents and accidents at DOE facilities. The main computers are the Digital Equipment Corporation's VAX-class machines configured to provide real-time data assimilation, model calculations, and analysis. Approximately one million lines of computer code have been written during the past four years to form the basis for this real-time system.

In addition to providing the base service to the DOE and the DOD, this group also focuses on improving and extending its capabilities. For example, our response to the Chernobyl accident led us to expand the scale of modeling from regional to global, and to assemble hemispheric wind field data sets from AFGWC every 12 hr. ARAC is now prepared to address in near real-time any accident in the northern hemisphere north of 20 degrees latitude. As time and resources permit, this capability will be extended to the southern hemisphere and tropical region to complete the development of a global response capability.

On the international scene ARAC has participated directly with other countries to help improve their emergency response systems and has worked with the nuclear safety directorate within the International Atomic Energy Agency. Staff members have helped review emergency response systems for developing countries and have participated in developing and writing Safety Series documents, which are guides (published in six languages) that recommend procedures to follow in order to meet certain safety standards. These particular Safety Series documents will be used by countries throughout the world as guidance for planning and implementing emergency response systems for nuclear facilities.

In the future we expect to begin investigating toxic-chemical emergency response capabilities and determining how they might be integrated into the ARAC structure. This expansion will be aided by the recent merger of the heavy gas group at LLNL into G-Division and the joining of our technical capabilities (see "Heavy Gases and Toxics"). This combined resource will provide a powerful tool for expanding the ARAC service to include toxic-chemical and heavy-gas emergency planning, response, and assessment activities.

Model Applications and Nuclear Effects Group

Role

The Model Applications and Nuclear Effects Group is responsible for the development and application of models to represent the release, atmospheric dispersion, and deposition of radionuclides, extending from generating source terms to estimating environmental and health effects.

Capabilities and Accomplishments

- Developed suite of models that can treat local to global dispersion and fallout of radioactivity.
- Performed detailed evaluation of the hemispheric dispersion of radioactivity released by the Chernobyl event and the venting of a U.S.S.R. underground weapon test.
- Continues to evaluate models against field studies.

Key Issues

- Integrated modeling capabilities across spatial/temporal scales.
- Increased focus on treatment of specific radionuclides.

Focus: This group focuses on developing models to represent the release, atmospheric dispersion, and deposition of radionuclides. Available models can be used to estimate the source term (amount, and time and space distribution of nuclear material), to simulate atmospheric transport and deposition, and to estimate environmental and health effects. The atmospheric modeling aspects are directly related to G-Division's major expertise of atmospheric model development. For source-term and dose-modeling expertise, we rely heavily on work outside the Division's mainstream research activities.

In the model application area, needs are identified and models are developed, improved, or changed to address these needs. One of the largest benefactors of this effort is ARAC. In ARAC's role as a federal emergency preparedness resource, many needs arise that require model modifications or additional development. For example, during preparation for and the reentry of the Soviet satellite Cosmos 954 over Canada in 1978, a major fraction of the thermonuclear power source broke up and dispersed radionuclides starting at about 40 km above Earth's surface. Models were modified to estimate the pattern of radioactivity that would reach the ground as a function of particle size. These calculations were used to help define the boundaries of an area where radioactive particles were removed from the surface of the snow. For the Gore, Oklahoma, UF_6 release in January 1986, a transport and diffusion model was modified to estimate concentrations and account for the chemical transformation of the material. Work is currently under way to include grid-point rainout in the models, include explosive dispersal directly as a "front-end" model, and develop a mesoscale forecast model for predicting wind and temperature fields.

To improve our estimates of nuclear effects, the major focus is on integration of capabilities that are required to assess the environmental impact (particularly health effects) resulting from an atmospheric release of nuclear material. The release of material can occur from events such as nuclear power plant accidents, satellite reentries, nuclear weapons accidents, or transportation accidents. One of the major tasks involves the development of methodologies and models that can describe the various potential source terms. Another task involves incorporating dose models into the chain of calculations so that we can estimate dose-to-man from a variety of different exposure pathways. The models can also be used to consider dispersion and deposition in studies of various nuclear war scenarios.

Mesoscale and Fluid Dynamics Group

Role

The Mesoscale and Fluid Dynamics Group is responsible for developing and applying advanced fluid dynamical models for use in mesoscale studies and for investigation of specialized problems.

Capabilities and Accomplishments

- Hierarchy of one-, two-, and three-dimensional finite-element models.
- Model application to: stably stratified flows, gravitational spreading of heavier-than-air gases, crystal growth, convection in liquid uranium, atmospheric flow in complex terrain (ASCOT).

Key Issues

- Development of mesoscale forecast model for ARAC.
- Support for continued numerical method advancement.
- Incorporation of more physics and chemistry into the heavy-gas model.
- Turbulence modeling.

Focus: The goals and activities of this group are threefold: development of new and better fluid mechanics (and transport/diffusion) models; application of existing models to current areas of interest/concern; and specialized support, both to other groups in the Division and to LLNL.

The mesoscale modeling efforts are divided into two major areas: nonhydrostatic and hydrostatic; and, because hydrostatic models are less expensive to run on the computer, part of the charter of the group is to better understand and describe those conditions under which the hydrostatic approach is an acceptably accurate approximation of the actual nonhydrostatic conditions. Our current mesoscale model is a nonhydrostatic finite-element model that is useful for simulating small-scale and/or locally driven phenomena such as drainage flow in complex terrain.

Several current fluid dynamics models that solve either the incompressible Navier-Stokes or Boussinesq equations, or the anelastic equations, also exist. These are also finite-element models and are (or have been) used to accurately compute isothermal flows (e.g., vortex shedding behind a cylinder), thermal convection flows (both in air and in other fluids, some a bit more exotic such as liquid uranium), stably stratified flows, and the gravitational spreading and dispersion of heavy gases such as liquefied natural gas (LNG).

Hydrostatic mesoscale models are currently under construction, both finite-element and finite-difference. One of these models will eventually be tailored to meet ARAC's needs and delivered to them to be used as a forecast model to replace their current persistence forecast assumption. Other versions of these models should find uses in both larger-scale studies of flows in complex terrain and for study of toxic releases that are of neutral or near-neutral buoyancy.

An evolving nonhydrostatic model is being used to simulate flow and heat transfer in high-temperature molten "glass." This finite-element model is also being applied to research and development applications for the laser program at LLNL in the area of new, high-quality optical materials that are grown from melts.

Planned support activities of this group for other groups in the Division are directed toward but not limited to: ARAC Operation and Assessments Group, Model Application and Nuclear Effects Group, Heavy Gas and Toxic Chemicals Group, and Atmospheric Microphysics and Chemistry Group. The Mesoscale and Fluid Dynamics Group has also been called upon in the past to provide computational fluid dynamics support to other (nonatmospheric/geophysical) programs at LLNL, and expects to do so in the future.

Heavy Gases and Toxics Group

Role

The purpose of the Heavy Gases and Toxics Group is to enhance, experimentally verify, and apply models that represent the atmospheric consequences of releases of heavier-than-air and toxic gases.

Capabilities and Accomplishments

- Verified, state-of-the-art heavy-gas dispersion models.
- Extensive databases from experimental releases of LNG, HF, NH_3, and N_2O_4.
- Development of Nevada Test Site (NTS) Spill Test Facility.

Key Issues

- Government versus industry responsibilities for funding accidental release research and the Spill Test Facility.
- Treatment of aerosols from phase transitions and chemically reactive spills.
- Interface into ARAC emergency response capability.
- Application of research results to federal, state, and local problems.

Focus: The Laboratory recently combined the Heavy Gases and Toxics Group (formerly J-Group, the Liquefied Gaseous Fuels Program) with G-Division. This group will continue to conduct research into heavy-gas dispersion and the consequences of accidental releases of hazardous chemicals into the atmosphere. Continued analyses of field test data, particularly for releases of liquefied natural gas (LNG), hydrofluoric acid (HF), and ammonia (NH_3), are allowing improvements to be made in our dense gas dispersion models and are providing an improved understanding of what happens when these materials are released into the atmosphere in large quantities. A major study for the U. S. Air Force on dispersion modeling includes model assessment, development of benchmark data sets, and development of a validation methodology. Over the last few years, our efforts in the model development area have produced two leading heavy-gas dispersion models, FEM3 and SLAB. The addition of a detailed description of the thermodynamics associated with two-phase (liquid aerosol and vapor) release to the atmosphere is planned for the SLAB (one-dimensional, quasi-three-dimensional) dense-gas dispersion model. Improvements planned for the FEM3 (three-dimensional finite-element) model will consider improved two-phase thermodynamics and a more advanced turbulence parameterization. All model improvements are tested thoroughly using field data from our various field tests.

The Laboratory's Liquefied Gaseous Fuels Program, the scientific support and direction for which are provided by the staff members of the Heavy Gases and Toxics Group, has been responsible for conducting essentially all of the large-scale field tests with hazardous materials done in this country. The Liquefied Gaseous Fuels (LGF) Spill Test Facility at NTS is a major DOE capability available for conducting large-scale experiments with hazardous materials. The Laboratory has developed an extensive instrumentation system to support tests conducted at the facility. In addition, the Laboratory has conducted both numerous large-scale tests with liquefied natural gas, HF, N_2O_4, and NH_3 at NTS over the past four years, and field experiments with hazardous and heavier-than-air materials over the last ten years. As a result of these studies, the Group has developed an extensive database with quite fine spatial and temporal resolution for use in model verification studies. (A more detailed discussion of the history and accomplishments of the LGF program can be found in Appendix E.)

The data archives from these tests provide a unique atmospheric dispersion data set in terms of their high temporal and spatial resolution, and this valuable resource can be used for further analysis and model validation. Participation in an emerging joint research program of the Department of Transportation (DOT)–DOE–EPA with industry is being sought. It is expected that more field testing will be conducted, but no firm commitments by industrial or governmental organizations have been made at this time to sponsor such work in fiscal year (FY) 1988 or beyond.

Atmospheric Microphysics and Chemistry Group

Role

The Atmospheric Microphysics and Chemistry Group is responsible for advancing the understanding of the physical, radiative, and chemical interactions of species injected into the lower atmosphere—generally shorter-lived, photochemically active species, which impact the boundary layer and troposphere on regional to global scales.

Capabilities and Accomplishments

- Detailed size-resolved aerosol/water drop microphysics model.
- Three-dimensional cloud and fire plume model.
- Regional photochemical air quality model.
- Global tropospheric model of nitrogen oxide transformations and budget.

Key Issues

- Development of three-dimensional global tropospheric chemistry model.
- Estimation of the role of electrical effects in fire plume scavenging.
- Treatment of ice physics in cloud model.
- Support for regional atmospheric chemistry studies.

Focus: The Atmospheric Microphysics and Chemistry Group is concerned with the physical, radiative, and chemical interactions of species injected into the lower atmosphere, generally shorter-lived, photochemically active species, which impact the boundary layer and troposphere on regional to global scales.

A major focus of this group is to study the fate of aerosols injected into the atmosphere. A detailed microphysics model has been developed that can treat the evolution of the size distribution of particles injected into the atmosphere (for example, smoke from post-nuclear fires) as they rise into a cloud and experience a supersaturated environment. In addition, two- and three-dimensional versions of an aerosol/cloud nonhydrostatic dynamical model have been developed for evaluation of cloud and precipitation development and the scavenging (removal) of aerosol from the atmosphere. Current model versions treat warm-rain processes, but they are being expanded to treat ice formation. They follow aerosol and aerosol-capture mechanisms through all phases of the precipitation process. Current applications involve the estimation of smoke scavenging above nuclear fires.

The group is also concerned with changes in the gaseous composition of the atmosphere. A three-dimensional photochemical transport model is being used to treat the transformation of urban and natural emissions, on scales up to several hundred kilometers. Current applications are focusing on the study of nitrogen transformation and export to the global troposphere and the role of nitrogen emission controls on urban and near-urban photochemistry. A global three-dimensional photochemical transport model has been developed to treat nitrogen oxide (NO_x) transformation to nitric acid and to evaluate the long-range transport and impact of anthropogenic NO_x emissions. Model validation and sensitivity studies are currently underway. Expansion to treat more complex photochemical cycles is planned.

We are also continuing to improve and further develop a hydrostatic regional/mesoscale model to treat cloud and fog formation and circulation responses to large smoke and aerosol injections. Our current focus is on evaluating changes in circulation patterns and the temperature response to large injections of smoke following a nuclear war. Our results indicate that the sharp initial cooling postulated in the "nuclear winter" hypothesis may be significantly ameliorated by fog formation.

Radiation and Global Chemical Interactions Group

Role

The Radiation and Global Chemical Interactions Group works to advance understanding of the radiative, chemical, and dynamical processes that determine the state of the global atmosphere, particularly with respect to the chemistry of longer-lived species injected into the atmosphere. Emphasis is on study of basic processes, the interactions of these processes, and comparison with observations.

Capabilities and Accomplishments

- Reference simulations for international assessments of chlorofluorocarbons, supersonic transports, nuclear weapons, etc.
- Science team members for Upper Atmosphere Research Satellite (UARS) project.
- One- and two-dimensional global chemical-radiative-transport models.
- One- and two-dimensional radiative transfer models.

Key Issues

- Coupling of two-dimensional chemical kinetics and climate models.
- Increased funding for chemistry-climate interactions studies.
- Extension of studies on effects of atmosphere on laser beam propagation.

Focus: Research in the Radiation and Global Chemical Interactions Group is aimed at studying the radiative, chemical, and dynamical processes that determine the state of the global atmosphere, particularly with respect to longer-lived species injected into the atmosphere that can mix upwards to the stratosphere and to global scales. Much consideration is given to studies of the interactions between the various processes. The models developed to study these processes and their interactions have been extensively used in national and international assessments of the effects that trace gases emitted into the atmosphere may have on the global distributions of ozone and temperature. Scientists in this group, as well as their research accomplishments, have also played major roles in the consideration of potential regulatory actions of trace gas emissions at both national (e.g., FAA, EPA) and international (e.g., United Nations Environmental Programme, Organization of Economic and Cooperative Development, World Meteorological Organization) levels.

For these studies, we have developed and are applying one- and two-dimensional radiative-chemical-transport models to study tropospheric and stratospheric processes. Our new two-dimensional model is a state-of-the-art tool for study of the complex atmospheric and chemical interactions brought on by injection of long-lived trace species. To aid in these studies, we are developing radiative transfer models to determine absorption and scattering properties of the atmosphere and their resultant effect on atmospheric temperatures. Analyses using the above models are being conducted to study the impacts that trace gases, including chlorofluorocarbons, CH_4, CO_2, and NO_x, will have on the global atmosphere. Past, present, and possible future states of the atmosphere are being examined with the models in an attempt to better determine existing limitations in our understanding of atmospheric processes and interactions. In support of the DOE's Carbon Dioxide Research Division, we are conducting studies, using the above models in collaboration with models of climatic processes, to examine the effects of trace gases on climate.

To assist in observational studies we are serving as science team members (as theoretical investigators) in the preparations for launch of NASA's UARS. After launch of this satellite (expected in FY 1991 or 1992), we expect to use the incoming satellite data and our models to improve our theoretical understanding of stratospheric and lower mesospheric processes.

Climate and Climate Change Group

Role

The Climate and Climate Change Group is responsible for advancing understanding of the factors affecting the climate, primarily those factors affecting atmospheric composition, by use of climate models and the comparison of model results with observational data.

Capabilities and Accomplishments

- One-, two-, and three-dimensional climate models of atmosphere and upper-ocean thermodynamics.
- Interactive climate–smoke simulations of nuclear war effects; identification of precipitation reduction effect.
- Responsibility for international general circulation model (GCM) and radiation model intercomparison projects.

Key Issues

- Funding for increased climate model diagnostics activities.
- Coupling of National Center for Atmospheric Research (NCAR)/CCM1 to vectorized smoke transport model.
- Development of coupled two- and three-dimensional ocean–atmosphere models for use in transient climate studies.
- Promotion and participation in DOE's Global Change program.
- Initiation of studies of planetary atmospheres.

Focus: The Climate and Climate Change Group studies the effects of changes in atmospheric composition on climate. Research ranges from study of the role of interactions between individual processes in affecting the climate (e.g., cloud interactions with solar and infrared radiation) to integrated studies of the effects of gaseous and aerosol changes on atmospheric and oceanic conditions.

A major effort is underway to understand why seemingly similar GCMs developed by different research groups generate different results (i.e., sensitivities to the same radiative forcing). The GCM comparison project that we coordinate involves many of the world's climate modeling groups, including ourselves, in a series of special simulations intended to determine the reasons that seemingly similar GCMs give different responses to the doubling of the CO_2 concentration. The present phase of the project, being directed in cooperation with scientists at the State University of New York (SUNY)/Stony Brook and Oregon State University (OSU), is looking at the role of clouds in affecting radiative fluxes, including the use of satellite data to assess model accuracy. To understand the effects of differences in the treatment of radiation calculations, we provide leadership for the Intercomparison of Radiation Codes in Climate Models (ICRCCM) project, which involves more than 60 research groups from around the world in a study to determine the accuracy of radiation calculations, especially as the CO_2 concentration is changed.

In cooperation with scientists at New York University, we are developing a two-dimensional, coupled, atmosphere–ocean model to study the role of the ocean in slowing the rate of climatic change that is being forced by the increasing atmospheric CO_2 concentration. Our two-dimensional climate model has also been used recently to study the relative climatic effects of volcanic injections into different latitude bands and during different seasons.

We also provide scientific advice and support to aid the headquarters staff of the DOE's CO_2 research program. This effort, which began about ten years ago, recently included the editing and

co-authoring of the state-of-the-art reports on projecting and detecting of CO_2-induced climate change.

Since the initial suggestion in 1982 that smoke from post-nuclear fires could affect the climate, we have been using our models to estimate the potential climatic effects of massive smoke injections from fires started by a nuclear war. We were the first group to treat moving smoke, to identify the sharp reduction in precipitation over land, and to extend interactive ocean-atmosphere calculations to study potential effects the year following the war.

The Physics Department's Institutional Research and Development (IR&D) program provides support for modifying and adapting GCMs developed originally at NCAR and OSU for our use in studies of CO_2-induced climate change, "nuclear winter," and, in the future, planetary atmospheres. These efforts are intended to help build the underlying framework for continued growth of our studies of global change.

Research Highlights

Several articles have been selected from work accomplished in the Division to illustrate the research activities that have been conducted during the past year. Appendix F provides a list of journal articles, book chapters, and conference presentations published in this time period.

The Use of the Øresund Experimental Data To Evaluate the ARAC Emergency Response Models

by Paul H. Gudiksen and Sven-Erik Gryning

Introduction

A series of meteorological and tracer experiments was conducted during May and June 1984 over the 20-km-wide Øresund strait between Denmark and Sweden for the purpose of (1) studying atmospheric dispersion processes over cold water and warm land surfaces, and (2) providing the data needed to evaluate mesoscale models in a coastal environment (Gryning, 1985). In concert with these objectives, the data from these experiments have been used as part of a continuing effort to evaluate the capability of the three-dimensional MATHEW/ADPIC (M/A) atmospheric dispersion model to simulate pollutant transport and diffusion characteristics of the atmosphere during a wide variety of meteorological conditions (Dickerson, 1985; Gudiksen, 1985). Since previous studies have primarily focused on M/A model evaluations over rolling and complex terrain at inland sites, the Øresund experiments provided a unique opportunity to evaluate the models in a coastal environment.

The Øresund experiments were conducted jointly by scientists from 16 institutions situated in Denmark, Finland, Norway, Sweden, Belgium, Germany, and the Netherlands (Gryning, 1985). The experiments included extensive meteorological measurements over an 80-km-wide cross section of the Øresund strait, as well as sulfur hexafluoride tracer studies for evaluating pollutant transport and diffusion processes. The locations of the meteorological measurements are shown in Fig. 2. These locations were selected on the basis of evaluating the expected spatial variability of the meteorological conditions associated with the upwind land area, the coastal zones, the water surface, and the downwind land area. The meteorological instrumentation included Doppler sodars, radiosondes, and meteorological towers (as shown in Fig. 2), as well as aircraft and boat-mounted meteorological and tracer instrumentation.

The tracer experiments involved the release of SF_6: (1) at a height of 95 m from the Barsebaeck meteorological tower, situated at location 10 (Fig. 2) along the Swedish coastline, during easterly winds, and (2) at a height of 115 m from the Gladsaxe meteorological tower, situated within the northern part of Copenhagen at location 4, during westerly winds (Lyck and Olesen, 1986). The tracer releases were generally conducted over four-hour periods, while time-averaged sampling was conducted over a one-hour period at specific sites along one or more arcs located on the downwind coastline and in inland areas. Instantaneous sampling was also performed by aircraft-, boat-, and van-mounted measurement systems. Nine tracer experiments were carried out; however, only six of these were judged to be suitable for this model evaluation study. Of the three remaining experiments, two were insufficiently covered by the tracer sampling arcs, and the tracer studies were cancelled during the third experiment due to unfavorable weather conditions.

Derivation of Model Input Values

The mean wind fields derived by the MATHEW model were based on the horizontal winds measured by the sodars and the meteorological towers (denoted in Fig. 2). These data were averaged hourly and interpolated to a three-dimensional grid mesh using 1-km horizontal and 30-m vertical

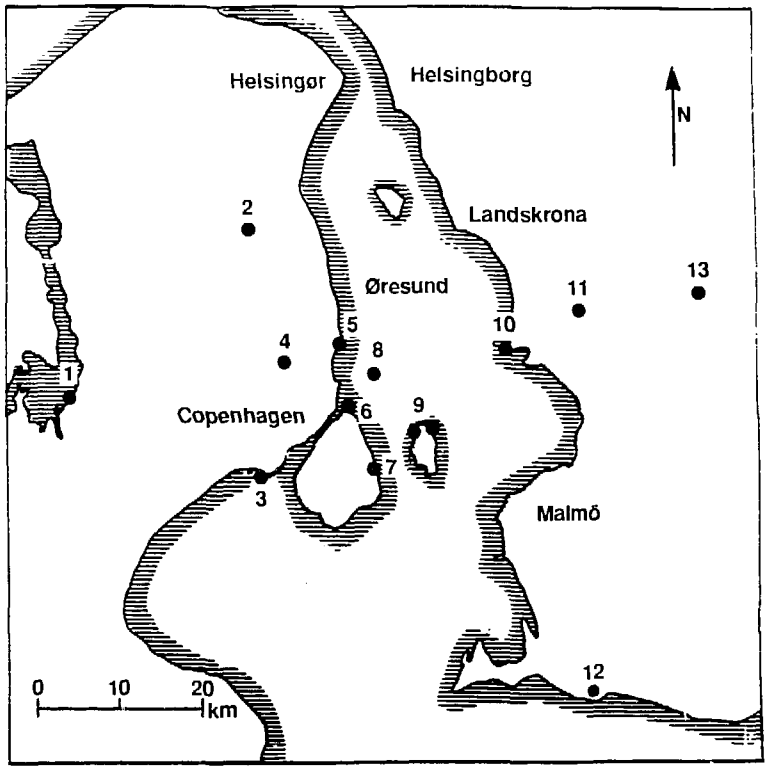

Figure 2. Layout of the meteorological instrumentation. The location numbers refer to (1) Riso, (2) Sjaelsmark, (3) Avedore, (4) Gladsaxe, (5) Charlottenlund, (6) Margretheholm, (7) Kastrup Airport, (8) Middelgrunden, (9) Saltholm, (10) Barsebaeck, (11) Furulund, (12) Maglarp, and (13) Borlunda.

grid spacing. The grid generally covered a 30-×50-km region extending across the Øresund strait up to a height of 480 m.

The horizontal diffusion characteristics of the atmosphere over land and water surfaces were estimated on the basis of σ_θ measurements made at the 95-m Barsebaeck tower and at the 115-m Gladsaxe tower, and on the basis of eddy dissipation rate measurements made at a height of 300 m by aircraft-mounted turbulence instrumentation (Sivertsen, 1986). The σ_θ data, in conjunction with the typical variation of σ_θ with height, permitted the construction of a vertical profile of σ_θ that extended to the top of the grid mesh over the land area (Brost et al., 1982). Since σ_θ values were unavailable over the water, the eddy dissipation rate measurements were used to extrapolate the σ_θ values from over land to over water. The values over water were typically 20–30% less than those over land.

The vertical diffusion characteristics of the atmosphere were based on the Monin-Obukhov scale length derived from the Barsebaeck tower measurements, the local friction velocities, and surface roughness heights.

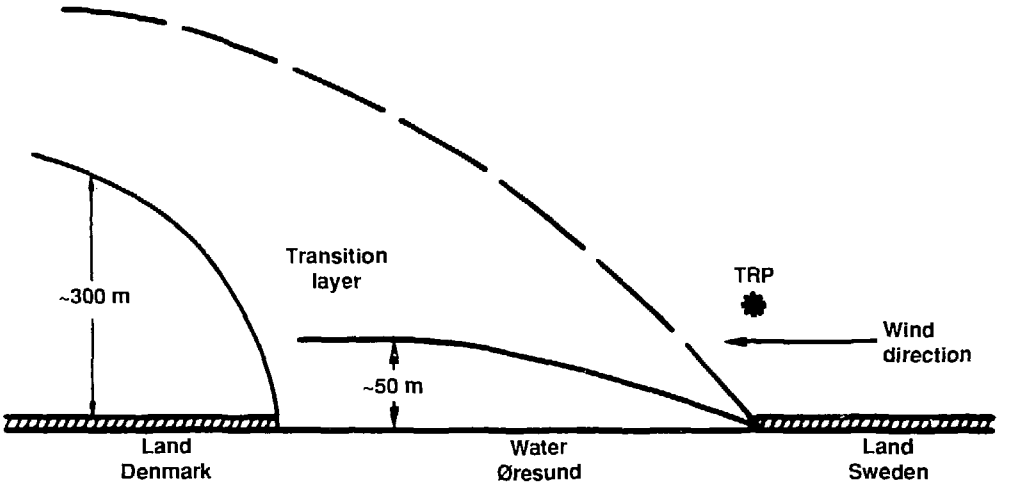

Figure 3. Generalized structure of the atmospheric boundary layer along east-west cross section of the Øresund strait. The **TRP** denotes the SF_6 tracer release point at Barsebaeck, Sweden.

General Meteorological Conditions under Study

The Øresund strait is a body of cold water that is capable of decreasing the surface air temperature by several degrees Celsius relative to that over the upwind land area. This decrease in surface temperature coupled with a change in surface roughness produces an interesting meterological situation. Analysis of the experimental data and numerical modeling by Doran and Gryning (1987) has revealed the general structure of the boundary layer over the water and adjacent land areas that is illustrated in Fig. 3. The figure depicts the case of air flowing in a westerly direction from southern Sweden, across the Øresund strait, and subsequently over the city of Copenhagen, Denmark; however, the illustration may readily be inverted for flows in the opposite direction. When the relatively warmer air over the Swedish land mass is advected over the surface of the Øresund strait, it encounters a shallow, stable surface layer that increases in depth as the air moves farther inland from the upwind coastline. Typically, the depth is 50–100 m in the vicinity of the downwind coastline (Batchvarova and Gryning, 1987). Due to the lower surface roughness over the water, the surface winds initially undergo an acceleration over the water immediately downwind from the coastline, but then decrease in speed as the stable layer over the water surface starts to act on the surface winds. As the wind encounters the heated Danish land mass, the increased mixing produces acceleration even though the surface roughness is substantially larger. Thus, a turbulent surface layer that increases in depth from the coastline is produced over the downwind land area. Its depth is typically about 300 m over Copenhagen at an inland distance of 5 km. Above these surface layers lies a transition layer that is initiated at the upwind coastline and typically increases in depth to as much as 500–700 m.

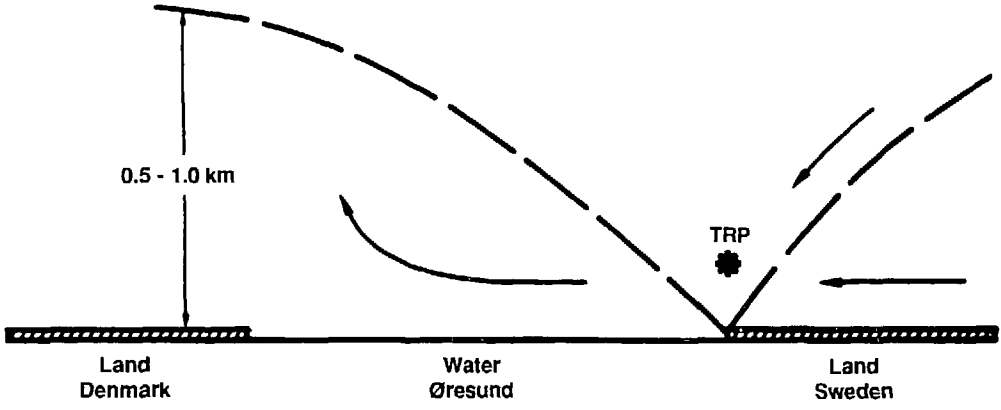

Figure 4. Generalized depiction of the atmospheric boundary layer flows along east-west cross section of the Øresund strait.

According to the modeling results of Doran and Gryning (1987), the initial acceleration over the water and the subsequent deceleration near the downwind coastline produce the characteristic flow field that is illustrated in Fig. 4. As the surface air initially accelerates, downward vertical motion is generated over a region near the upwind coastline. This is followed by upward motion caused by the deceleration near the downwind coastline.

These surface-boundary-layer characteristics have profound effects on the dispersion of pollutants entrained within these layers. These become more apparent in the course of the M/A model simulations, which follow the dispersion of the SF_6 tracer released near the upwind coastline during the Øresund experiments.

Results

Results of the M/A model simulation of the May 29 tracer experiment, along with a comparison with the measured SF_6 concentrations, illustrate the character of the flows, as shown in Fig. 5. The figure includes a plot of the calculated plume surface-air concentrations of SF_6 with the location of the sampling arcs superimposed. Also included is a direct comparison between the calculated and the measured SF_6 concentrations along each sampling arc. A review of the figure reveals that the calculated maximum concentration is higher than that measured, by a factor of four. In general, similar results were obtained for the other simulations.

The general over-prediction by the M/A models of the SF_6 concentrations probably reflects the meteorological processes described in Figs. 3 and 4. The SF_6 that was released into the transition layer was initially subjected to a slight downward motion as it was transported across the upwind coastline (see Fig. 4). This was borne out by vertical profile measurements of tracer concentrations over the Øresund during one experiment (Gryning, 1985). These measurements revealed that the maximum concentrations occurred at a height of 50 m, which was about 50 m below the release height. Thus, most of the tracer was situated immediately above the stable surface layer. The stable layer over the water undoubtedly tended to minimize mixing of the tracer into it, and, finally, the fraction that did become entrained within the stable layer was subjected to upward vertical motion as the surface air decelerated near the downwind coastline. The combined effects of these processes tended to reduce the surface air concentrations measured along the downwind coastline relative to those expected in the absence of the stable layer. Because the M/A models do

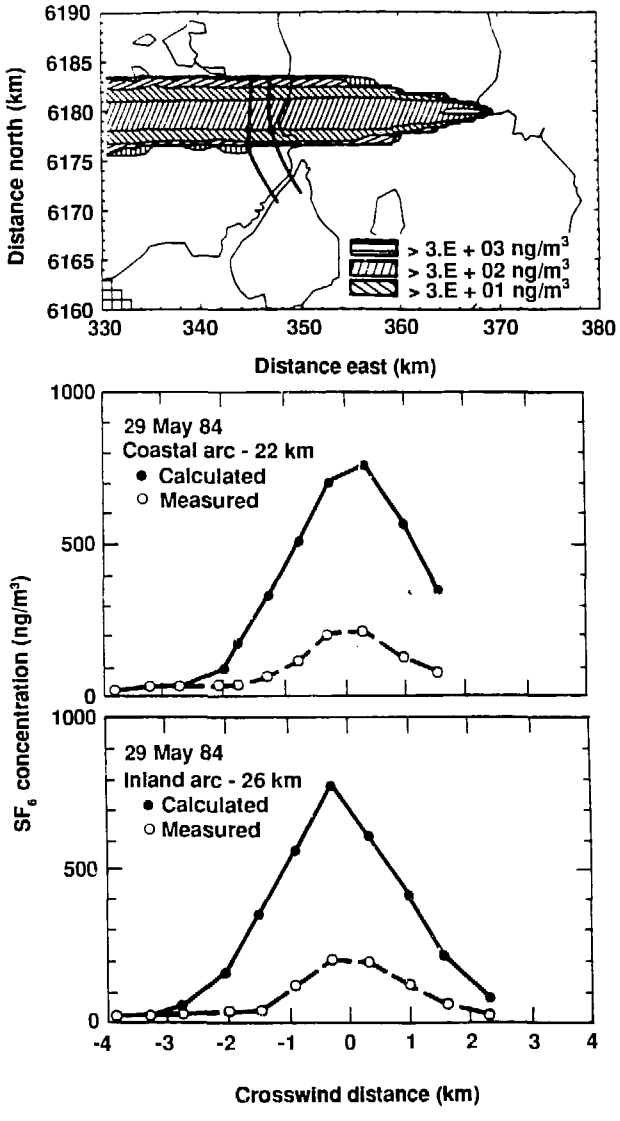

Figure 5. The calculated plume concentration pattern with the position of the sampling arcs overlaid (top figure), and a comparison of the calculated and measured concentrations along the coastal arc (middle figure) and the inland sampling arc (bottom figure).

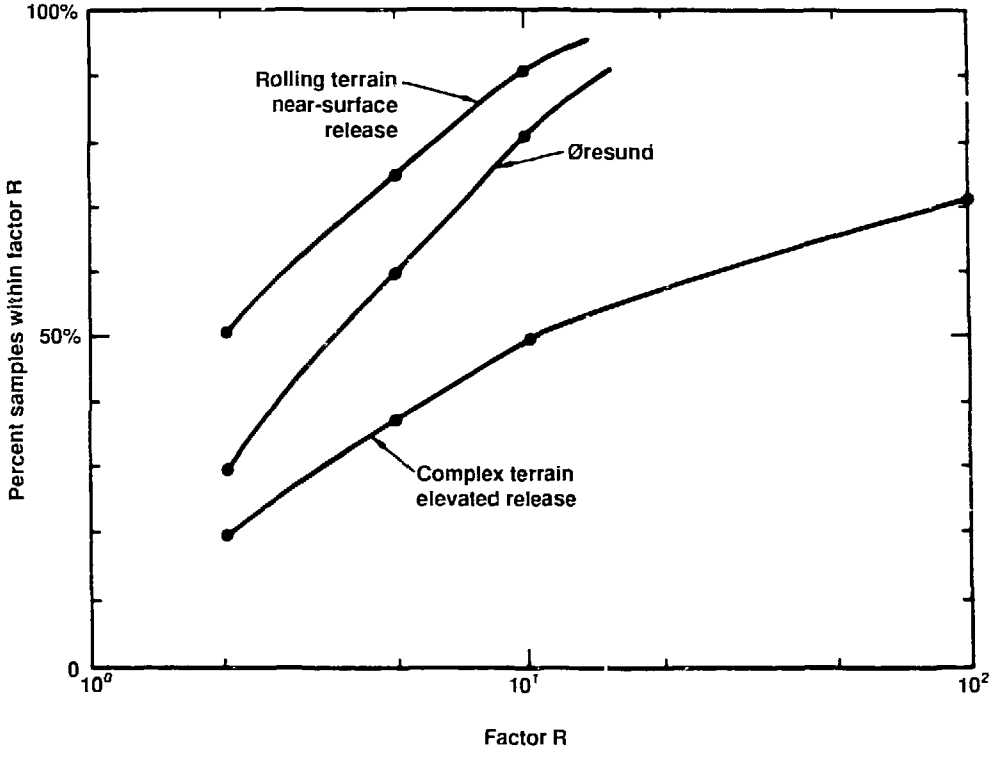

Figure 6. Percentage of computed samples within a factor R of measured tracer concentrations. The middle curve represents the results using the Øresund data, while the other curves represent the range of values derived from previous studies in rolling and complex terrain.

not have the capability for including the effects of this stable layer, the calculated concentrations are expected to be higher than those measured.

A statistical analysis of the performance of the M/A models was performed by deriving the factor R, which is the ratio of the calculated to the measured SF_6 concentrations at each sampler location for all six experiments. The factor is always greater than unity because its reciprocal is used if the ratio is less than unity. The results, given in Fig. 6, show the percent of the samples that are within any given factor R for about 130 comparisons. Thus, approximately 50% of the sample comparisons are within a factor of four. This may be compared with the range of results, also shown in Fig. 6, acquired during previous M/A model evaluation studies over rolling and complex terrain sites for both surface and elevated tracer releases. The previous results indicate that the factor

R values, derived from the Øresund study, fall within the range of results obtained from previous studies. The major difference, however, is that in this study the M/A models over-predicted the surface air concentrations, whereas no bias was detected in the previous studies.

On the basis of the results of this model evaluation study using the Øresund experimental data, we believe that in order to significantly improve our capability to simulate the dispersion of the SF_6 tracer across the Øresund strait, it is imperative that a three-dimensional model be used that explicitly incorporates the dynamical processes depicted in Figs. 3 and 4. Thus, the model must develop wind fields across the Øresund strait that include the effects of thermal stability as well as describe the turbulence characteristics that are responsible for mixing the tracer within and across the various surface boundary layers.

Model Evaluation Studies: Cross-Appalachian Tracer Experiment

by Daniel J. Rodriguez

In the fall of 1983, a field campaign, referred to as the Cross-Appalachian Tracer Experiment (CAPTEX), was launched under the joint sponsorship of several U. S. and Canadian agencies (Ferber and Heffter, 1984). Its main objectives were to test the tracer technology for transport and diffusion studies out to 1000 km and more, to provide data for evaluating and improving numerical models that simulate the transport of pollutants, and to provide insights into the mechanisms of atmospheric transport and dispersion. These data, offered freely to the modeling community, proved to be an excellent resource for testing our MEDIC and ADPIC models on the regional scale.

The experiment consisted of seven tracer releases—five at Dayton, Ohio, and two at Sudbury, Ontario—performed within a six-week period beginning in mid-September. The tracer, which was evaporated before its release at ground level, was a nontoxic, nonreactive perfluorocarbon (PMCH) having an ambient background of approximately four parts in 10^{15} parts of air. Such a minute background allowed meaningful measurements to be made out to great distances. Favorable release periods were selected, based on forecasts, to improve the efficiency of the tracer collection by a fixed array of ground-based receptors. More than 80 automatic sequential air samplers were strategically positioned throughout the northeastern U. S. and southeastern Canada. Sampling intervals, typically six hours, were generally short enough to document the arrival and departure of the plume in the absence of lofting. The placement of samplers along a series of arcs with a sampler spacing of approximately two plume standard deviations, usually guaranteed the detection of the PMCH at two or more sites along an arc during the passage of the plume. The disposition of the rawinsonde stations, which provided the bulk of the meteorological data, and the receptors in relation to the sources at Dayton and Sudbury are shown in Fig. 7.

Lawrence Livermore National Laboratory, along with other organizations, including the Tennessee Valley Authority, the National Oceanic and Atmospheric Administration's Air Resources Laboratory, and the Atmospheric Environment Service of Canada, subjected their model results to a battery of statistical tests (most of which were graphical in nature) devised by the Argonne National Laboratory. The graphical measures of performance, including histograms, cumulative frequency plots, and box plots, were designed to elucidate the strengths and weaknesses of long-range transport models. The most rigorous tests compared the observed and predicted concentrations in both space and time. Figure 8, a frequency histogram of the residuals (observed minus predicted concentrations), is an example of one such test. Basically, the residuals were symmetrically distributed about the zero point with exactly half of the values lying on either side. The frequency distribution of observed versus predicted concentrations unpaired in space and time is shown in Fig. 9 and, as might be expected, indicates a dramatic improvement. The use of unpaired statistics removes any performance penalties caused by wind speed and wind direction errors that enter the model. This test is an appropriate measure of performance when, for example, an analyst is most interested in a model's ability to predict peak concentrations.

From these and other results, several major conclusions concerning the ability of our models to simulate the long-range transport of airborne pollutants can be drawn:

- Peak concentrations are typically underestimated by a factor of 2 as the result of over-dilution of the pollutant mass by ADPIC along the sampling arcs nearest the sources.
- With the exception of peak concentrations, no systematic tendency exists for either over- or under-prediction by the model.
- Performance statistics deteriorate when the observations and predictions are paired in time and space, mainly as the result of misalignments of the plume centerline.
- Our treatment of diffusion (subgrid-scale eddy mixing) is excellent as suggested by the symmetry in the distribution of residuals.

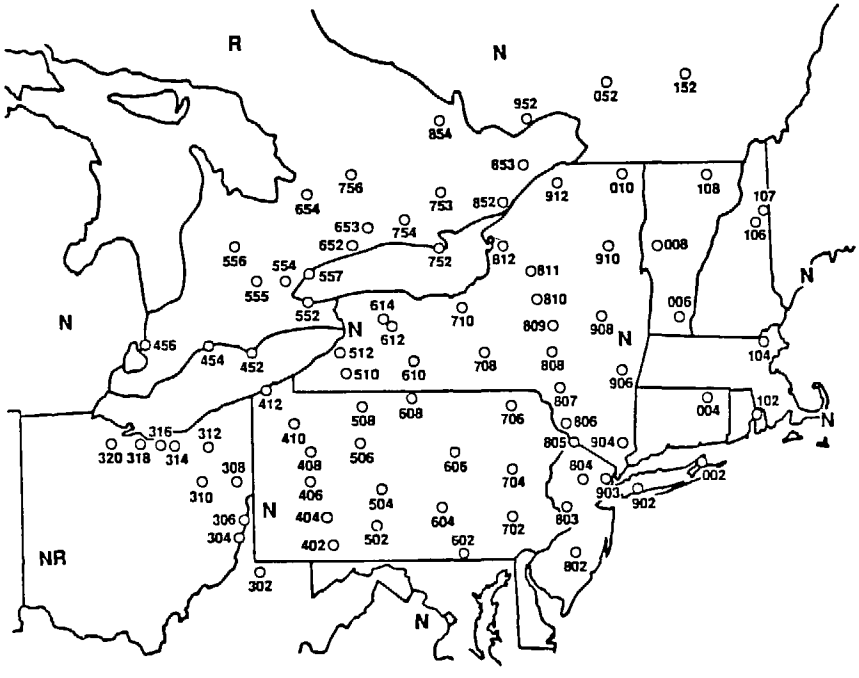

Figure 7. CAPTEX release sites (**R**), surface sampling sites (circles with numbers), and rawinsonde stations (**N**).

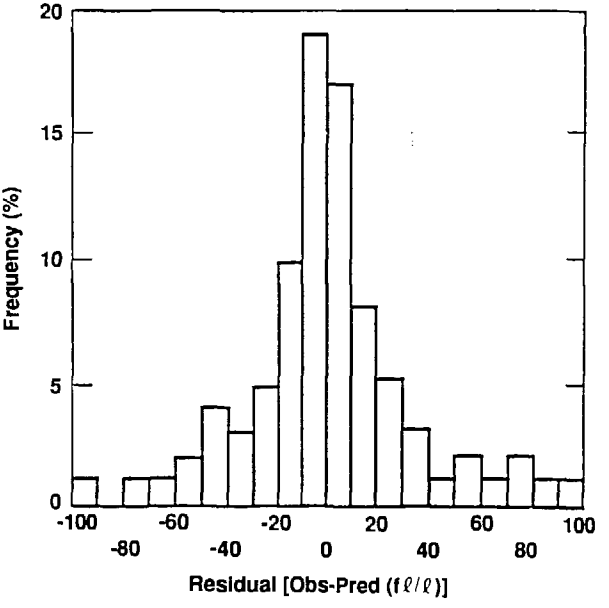

Figure 8. Frequency distribution of the observed minus predicted concentrations for values paired in time and space for all CAPTEX experiments.

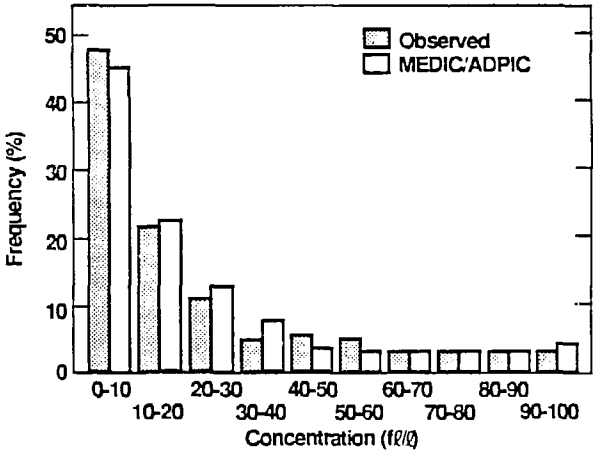

Figure 9. Frequency distribution of the observed and predicted concentrations for values unpaired in time and space for all CAPTEX experiments.

The Long-Range Transport of Nitrogen Oxides and Their Impact on Urban Photochemistry

by Joyce E. Penner, Peter S. Connell, Patrick P. Weidhaas, Daniel J. Rodriguez, and Cynthia S. Atherton

A major project in the Division during FY 1987 was completion of the development of a three-dimensional photochemical transport model for the treatment of urban photochemistry on regional scales (Penner and Connell, 1987). The development of this model was motivated by a need to understand the impact of urban emissions from the San Francisco Bay Area on downwind locations. In particular, the effect of NO_x emissions and emission control strategies on ozone exceedances in Monterey were evaluated.

Effect of NO_x Emissions on Photochemical Smog

Nitrogen oxide emissions are an essential component of photochemical smog. They, together with nonmethane hydrocarbons, act to form ozone and other photochemical oxidants in the presence of sunlight. However, increases in NO_x can also slow the photochemical process by decreasing the concentrations of HO_x and RO_x radicals. Furthermore, locally, near sources of NO_x, the reaction of NO with O_3 decreases O_3 directly.

In former studies of smog formation in the San Francisco Bay Area, an emission control strategy was adopted that sought to control only the emissions of nonmethane hydrocarbons while generally leaving NO_x emissions unchecked. However, because the dominance of reactions that tend to reduce the build-up of ozone would decrease with distance from the main urban centers in the San Francisco area, it was not at all clear that such a policy was beneficial to downwind areas. The purpose of this project was to evaluate the effect of this emission control strategy on ozone formation in Monterey.

Development of a Three-Dimensional Photochemical Transport Model

The code used previously by the Bay Area Air Quality Management District, the LIRAQ model, was a single-layer, photochemical transport model. Because this application required consideration of a two-day episode, it was necessary to develop a full, three-dimensional model in order to properly simulate the transport of pollutants above the boundary layer. Furthermore, the expanded region of interest (from a 100-$\times$100-km^2 to a 200-$\times$200-km^2 area) required development of a fast but accurate numerical technique. Therefore, in addition to providing the framework to be fully three-dimensional, a series of model improvements was made.

First, the solution technique was changed from that of the Gear method to one of operator splitting. Careful checks assured that the new numerical technique would perform as accurately as the previous, accurate Gear method. The operator splitting method was approximately twice as fast as the original technique.

Second, after testing several different techniques, the one developed by Smolarkiewicz (1983) was selected. This technique calculates the amount of numerical diffusion resulting from simple upstream differencing and corrects the advected species concentrations so as to remove that artificial numerical diffusion.

In addition, improvements to the MATHEW model were developed to specifically account for the presence of a boundary layer and the fact that flow should be restricted across the boundary. This model takes observed winds, interpolates them to produce a grid-wide wind field, and then adjusts the winds using a minimal adjustment technique to produce a field that is mass-consistent.

Evaluation of the Effect of NO_x Controls on Ozone Exceedances in Monterey

The improved model was used to simulate a two-day smog episode in the San Francisco Bay Area and Monterey. To accomplish this, the Bay Area Air Quality Management District (BAAQMD) developed an emissions inventory for nonmethane hydrocarbons, including representation of biogenic hydrocarbons, nitrogen oxides, and carbon monoxide, that was appropriate to the period of interest (September 30 and October 1, 1980) and had a spatial extent that encompassed the Monterey Bay Unified Air Pollution Control District. The BAAQMD also gathered the relevant meteorological data for that time period and used the improved version of the MATHEW model to developing wind fields appropriate to those two days.

The new model accurately predicted ozone formation over the new region for the case day. Figures 10 and 11 display scatter plots of the predicted ozone concentrations versus the observed concentrations at all stations and hours within the model domain. The comparisons showed an accuracy equivalent to previous model and observation comparisons, even though little to no tuning of the simulated meteorology was allowed. Furthermore, the model predicted a previously unexpected feature—the occurrence of an O_3 bulge off the western coast of the San Francisco peninsula (see Fig. 12). This bulge was also apparent in airplane observations taken during the study period, but had not been seen in previous model applications. As shown in Fig. 12, the existence of two transport paths for pollutants from the San Francisco area to the Monterey area was evident in the model simulation: one route over the ocean and one route along the Santa Clara Valley.

Finally, the effect of controlling the NO_x emissions was tested. Figures 13 and 14 show the effect of a 30% decrease in NO_x emissions in the Bay Area. The results indicated that ozone is substantially increased by control of NO_x in the area between San Jose and Hollister. This finding is consistent with previous model studies in the Bay Area using the LIRAQ model. However, the ozone bulge over the Pacific is reduced when NO_x emissions are decreased. Thus, there appears to be a small benefit to downwind areas when NO_x emissions are reduced. This result is, of course, limited to the particular meteorology studied. Furthermore, because the benefit to downwind areas is so small, it is also highly uncertain. The size and magnitude of the expected ozone change might change considerably with improved representations of the emissions inventory, the meteorology, and the chemistry in the model.

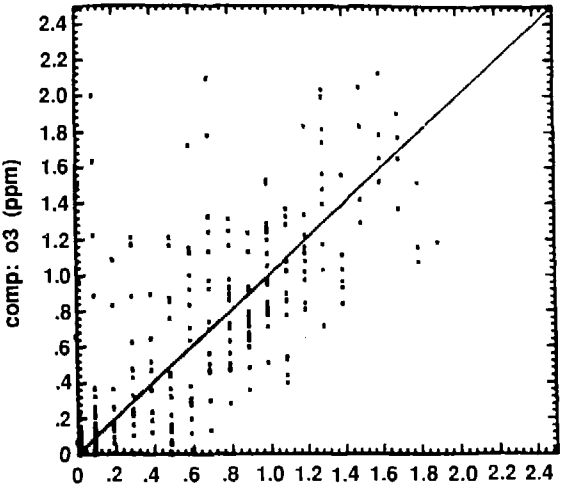

Figure 10. Scatter plot of computed and observed surface ozone concentrations on September 30, 1980. The comparison includes all stations and all hours for which data were collected within the 200-×200-km^2 grid.

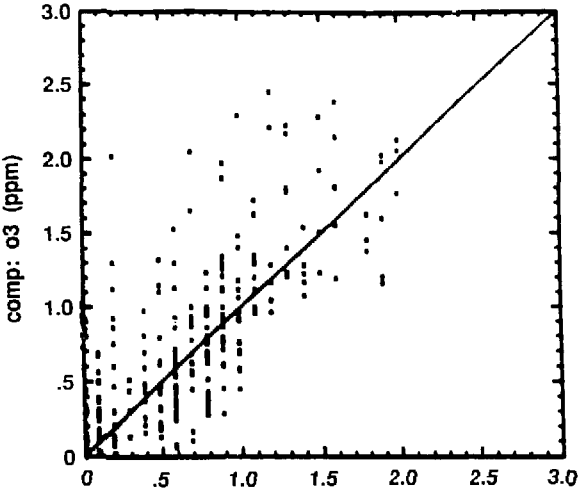

Figure 11. Scatter plot of computed and observed surface ozone concentrations on October 1, 1980. The comparison includes all stations and all hours for which data were collected within the 200-×200-km^2 grid.

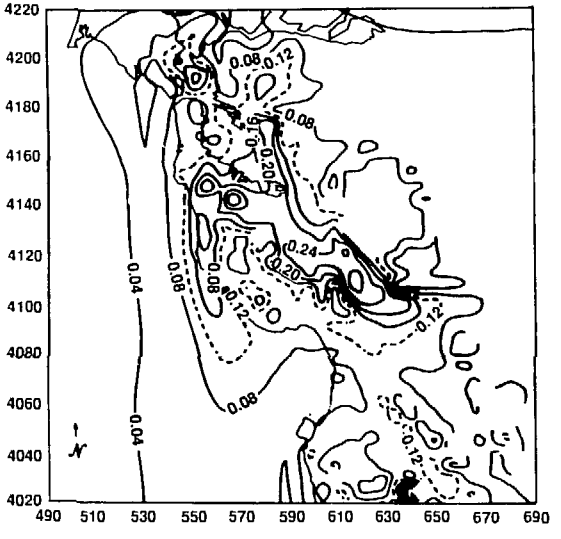

Figure 12. Predicted layer-average ozone concentrations within the mixed layer at 1600 hours on October 1, 1980. Contour units are ppm. Note the bulge in O_3 concentration off the coast of Monterey, showing the effect of the transport of pollutants from the San Francisco Bay Area out over the ocean and along the coast towards Monterey.

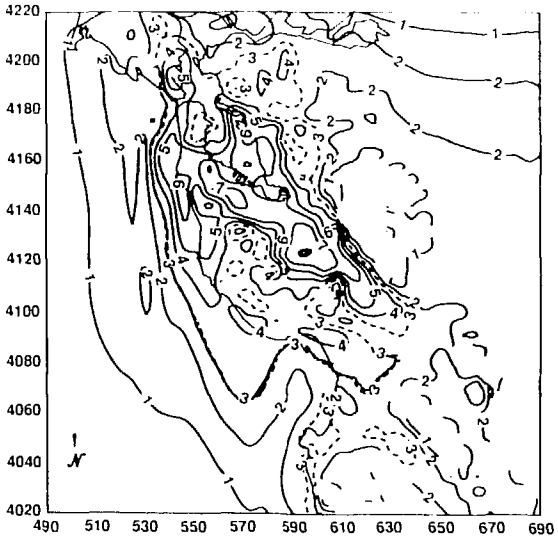

Figure 13. Predicted layer-average ozone concentrations for 1500 hours on September 30, 1980. Units are 1×10^{12} cm^{-3}. The dotted line corresponds to a layer-average concentration of about 0.12 ppm. All concentrations above that level are above the federal standard.

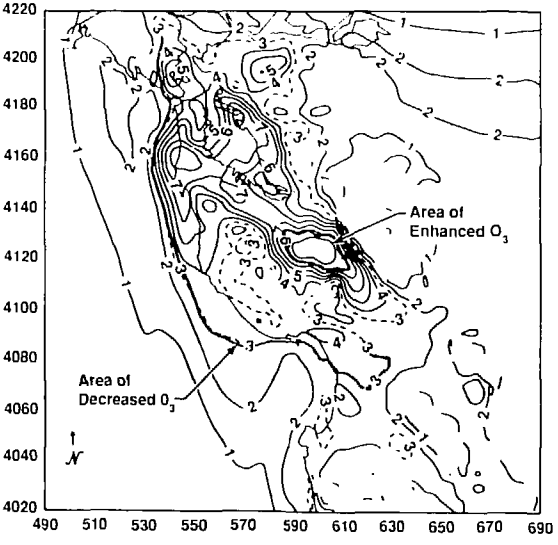

Figure 14. Predicted layer-average ozone concentrations for 1500 hours on September 30, 1980, for a case in which all NO_x emissions in the Bay Area Air Quality Management District were reduced by 30%. Ozone concentrations south of San Jose are generally increased, while further downwind and over the ocean, the O_3 concentrations decrease slightly.

Dose Estimates from the Chernobyl Accident

by Rolf Lange, Marvin H. Dickerson, and Paul H. Gudiksen

The Lawrence Livermore National Laboratory's ARAC Group responded to the Chernobyl nuclear reactor accident in the Soviet Union by utilizing long-range atmospheric dispersion modeling to estimate the amount of radioactivity released (source term) and the radiation dose distribution (due to exposure to the radioactive cloud) over Europe and the Northern Hemisphere (Dickerson et al., 1983). In later assessments, after the release of data on the accident by the Soviet Union (U.S.S.R., 1986), the ARAC team used their mesoscale-to-regional-scale model to focus in on the radiation dose distribution within the Soviet Union and in the vicinity of the Chernobyl plant.

The source term estimation involved an iterative process whereby an initial unit source term was used to calculate the distribution of radioactivity. These calculations were then compared with measurements of airborne radioactivity at about 20 sites throughout the Northern Hemisphere. Scaling of the calculated activity distributions with those measured led to an estimate of the total amount of radioactivity released as a function of time and its initial vertical distribution in the atmosphere. By using this source term, it was possible to calculate the spatial and temporal evolution of the radioactive cloud over Europe and the Northern Hemisphere and the inhalation radiation dose due to cloud exposure (Gudiksen and Lange, 1986).

Measurements of airborne radioactivity over Europe, Japan, and the U. S. detected the presence of fresh fission products up to heights of about 7 km within a few days after the initial explosion. These results strongly suggested that some of the radioactivity released by the explosion and the subsequent fire within the reactor core must have been transported to heights well within the middle troposphere. This high altitude presence of the radioactivity may have been due to a variety of factors such as the thermal energy associated with the releases and/or meteorological transport due to convective activity or isentropic up-gliding over a frontal system. Whatever the cause, the source term arrived at in the calculations consisted of an upper- and lower-level cloud of radioactivity. The upper cloud, centered at 4500 m and extending vertically from 1500 to 7500 m, was assumed to be due to the initial explosion; the lower cloud, centered at 1300 m and extending from the surface to 1500 m, was assumed to be produced by the hot fire that continued to cause radioactive emissions for six days after the initial explosion. This combination of radioactive emissions indicated that 50% of the radioactivity was released in the upper cloud during the first day of the accident, and the remaining 50% was released over a six-day period in the lower cloud that resulted from the ensuing fire.

Using these emission rates, a three-dimensional particle-in-cell atmospheric dispersion model that was specifically adapted to treat continental and hemispheric spatial scales was employed for this analysis (Lange, 1978b). In the model, several marker particles were injected at the source point to represent the radioactivity. The particles were subsequently transported within a three-dimensional grid mesh by the winds, atmospheric diffusion, gravitational settling, and dry deposition. The calculations were based on a computational mesh covering the Northern Hemisphere, with a smaller-particle sampling grid placed over Europe for increased spatial resolution. The Northern Hemispheric wind fields used by the model were provided by the U. S. Air Force Global Weather Central (AFGWC), and the rate of diffusion was estimated by assuming a neutral to slightly unstable atmosphere. This model does not directly test the effects of rainout since rainfall data on the Northern Hemispheric scale are not available. However, since the results are scaled to radiological measurements obtained throughout the Northern Hemisphere, rainout is included implicitly.

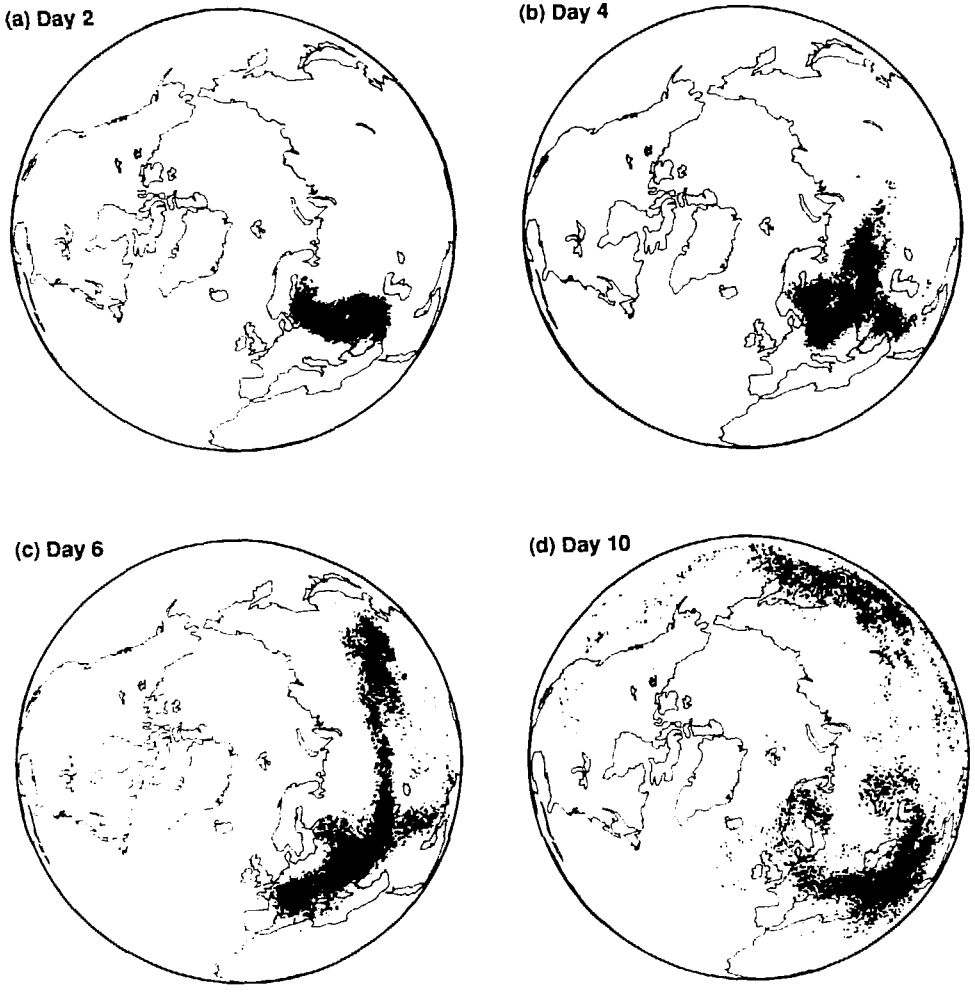

Figure 15. ARAC plots showing how the clouds of radioactive material spread around the Northern Hemisphere at (a) 2, (b) 4, (c) 6, and (d) 10 days after the initial explosion.

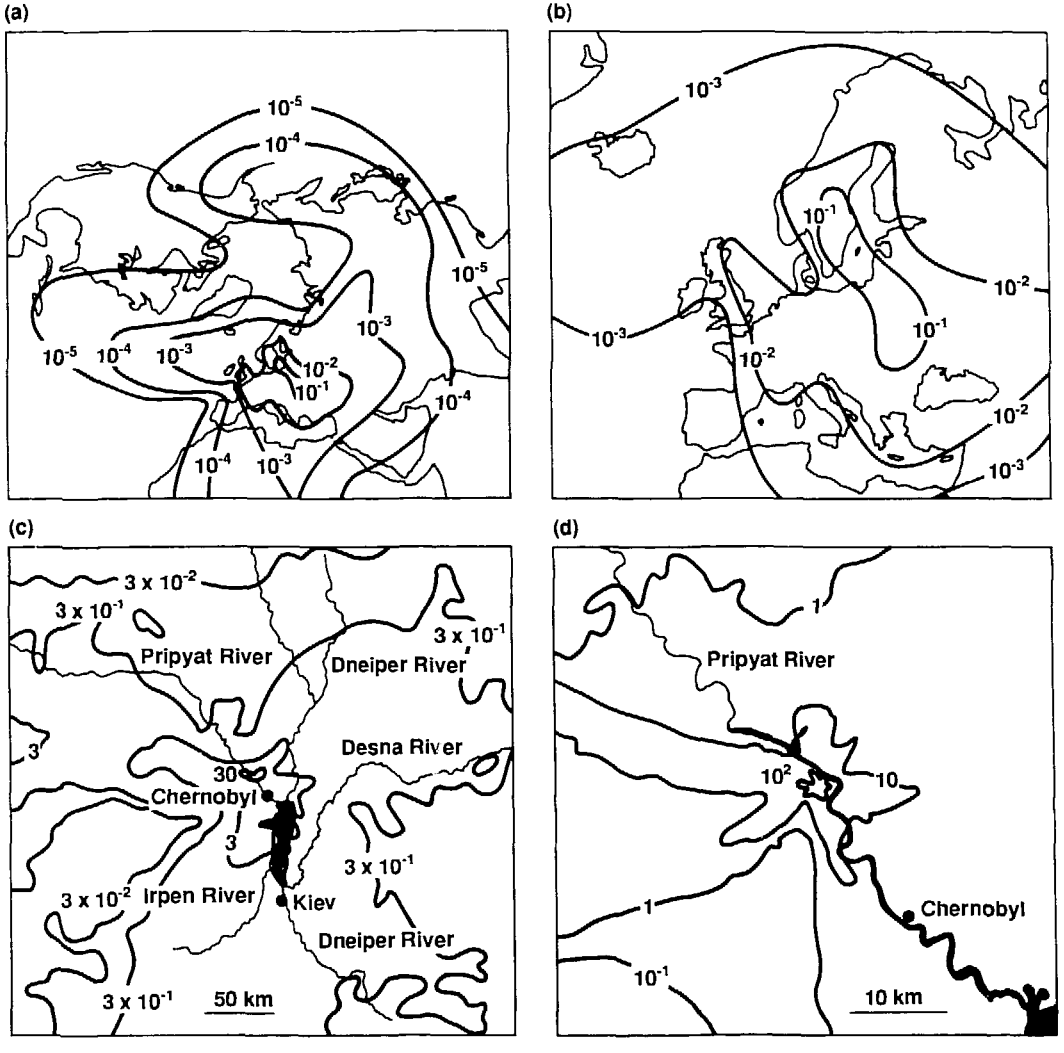

Figure 16. Isopleths showing the distribution of cumulative primary radiation dose (that due to breathing the contaminated air, integrated over the next 50 years). The isopleth values are given in mGy. (a) Most of the Northern Hemisphere, in a modified polar projection. (b) Europe, the Mediterranean Sea, and the North Atlantic. (c) A 400- ×400-km area around the Chernobyl reactor. (d) A 50- ×50-km area around Chernobyl. The values for the isopleths increase slightly as the scale decreases because our computer models achieve finer resolution at smaller scales.

Analysis of the airborne radioactivity distribution indicated that the cloud became segmented during the first day, with the lower section heading toward Scandinavia and the upper part heading in a southeasterly direction with subsequent transport across Asia to Japan, the North Pacific, and the west coast of North America (see Fig. 15). Integrating these concentration distributions over the period from April 26 to May 13 produced the unmitigated individual inhalation and immersion dose distributions due to exposure to the airborne radioactivity over Europe and the Northern Hemisphere.

Figure 16 shows the computed isopleths for the total committed effective dose equivalent to an adult due to inhalation alone. (The external and internal doses due to deposited radionuclides can be very important sources, especially when no mitigative measures are taken.) The contours show a distribution pattern in Europe of a region where the dose exceeds 100 μSv (10 mrem) extending over the western U.S.S.R., northeastern Poland, and up into Sweden, while extending southward over the Ukraine and parts of eastern Europe. Most of central Europe, parts of northern Scandinavia, and the remainder of eastern Europe are situated between the 10-μSv (1-mrem) and 100-μSv (10-mrem) isopleths. Denmark, the United Kingdom, Spain, and northern Scandinavia received less than 1 μSv (1 mrem). About 80% of these values are due to radioiodine, while the cesium, ruthenium, and tellurium radionuclides are the major contributors to the remaining 20%.

Because the spatial distributions for immersion in the radioactive cloud are essentially identical to those for inhalation, one may obtain the corresponding effective dose equivalent by multiplying the isopleths by approximately 0.02. Because of the large spatial averaging inherent in these calculations, the radiation doses are greatly underestimated in the vicinity of the Chernobyl area. Figure 16 also shows a more detailed assessment, based on a close-in calculation with the ARAC mesoscale-to-regional-scale ADPIC model (Lange, 1978a) centered on the reactor site, which revealed total inhalation doses from 300 μSv (30 mrem) at distances of 200 km, to values of above 43 mSv (2 rem) near the plant over the first 10 days after the accident. While close to the accident site the doses are dangerously high, for Europe the individual dose commitment is equivalent to that normally received from background radiation in a few years. For the rest of the Northern Hemisphere the effects are minimal.

The LLNL Two-Dimensional Model of Global Atmospheric Chemistry: Past Trends in Ozone

by Donald J. Wuebbles and Douglas E. Kinnison

The newly developed LLNL two-dimensional chemical-radiative transport model of the troposphere and stratosphere (Wuebbles et al., 1987) has been applied to an analysis of the effects that natural and anthropogenic influences may have had on global ozone concentrations over the last three decades. This model currently calculates the time-dependent zonally averaged concentrations of more than 30 relevant atmospheric constituents as a function of latitude and altitude. Full seasonal variations are included. Approximately one hundred chemical and photochemical atmospheric reactions are included in the model. Transport of trace species in the troposphere and stratosphere is determined by using the diabatic-driven winds derived from model-calculated net radiative heating rates. These heating rates are calculated in an internally consistent way using derived species distributions. Subgrid-scale eddy mixing is parameterized assuming a diffusive representation.

Emissions and atmospheric concentrations of several trace gases important to global atmospheric chemistry are known to have increased substantially over recent decades. Anthropogenic influences are thought to be primarily responsible for the observed increasing concentration of CO_2, CH_4, N_2O, and several chlorofluorocarbons. Variations in ultraviolet radiation during the 11-year

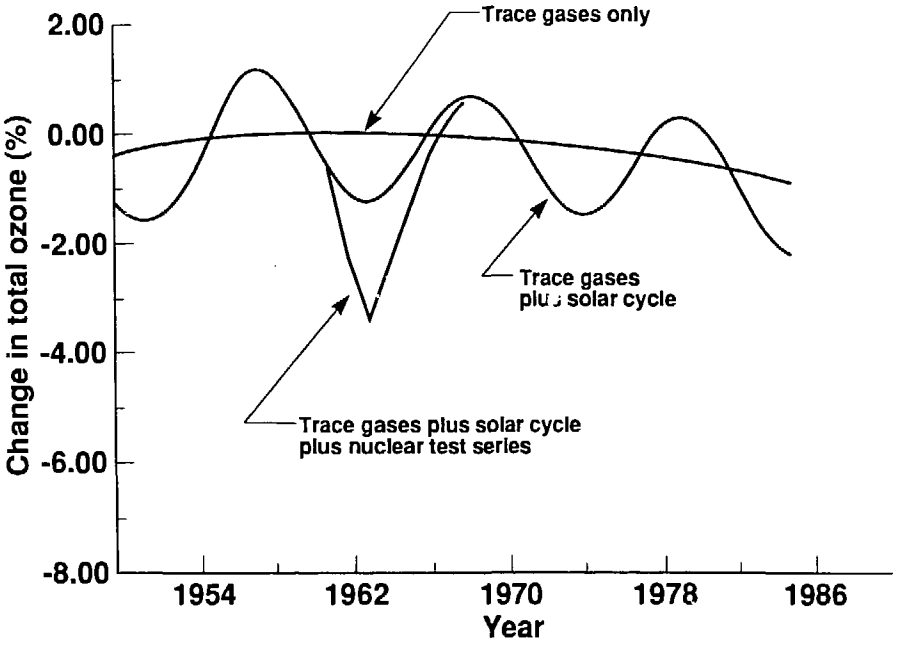

Figure 17. Past trends in globally and annually averaged total ozone as computed in the LLNL two-dimensional model of the troposphere and stratosphere.

solar cycle are likely to influence upper stratospheric photochemistry. The U.S. and U.S.S.R. atmospheric nuclear test series of the late 1950s and early 1960s may have produced enough NO_x to affect stratospheric ozone concentrations.

In modeling past trends, estimates for historical changes in trace-gas surface emissions and concentrations, variations in ultraviolet radiation, and NO_x emissions from nuclear tests were used as model inputs to examine the calculated changes in ozone since 1950. Available measurements and published analyses were used in the derivation of these inputs.

In general, the resulting model-calculated tropospheric and stratospheric distributions of ozone and other trace species for the current atmosphere agree well with available land- and satellite-based observations. However, there are also indications, such as in the underestimation of winter high-latitude stratospheric amounts of nitric acid, that current theoretical understanding of global atmospheric chemistry is still incomplete.

The calculated trends in the globally averaged total ozone column for the assumed historical variations are shown in Fig. 17 for three cases. The first case considers the expected effect if only trace gas emissions of chlorofluorocarbons (e.g., $CFCl_3$, CF_2Cl_2), methane (CH_4), and nitrous oxide (N_2O) were assumed to be responsible for changes in ozone over the last 35 years. The second case adds in the effects of assumed changes in solar flux during the 11-year sunspot cycle, while the third case also includes the effects on ozone of NO_x injections from atmospheric nuclear testing.

According to our study, only a small change in total ozone would be expected due to trace gases over this period, but a 2% global decrease in total ozone would have been expected in the early 1960s due to nuclear tests. The change in total ozone determined from solar maximum to

solar minimum varies with the specific solar cycle, but is approximately 2% for the current cycle. These results are in good agreement with available ground-based Dobson measurements of total ozone. The calculated decrease in total ozone since 1978 of about 2%, primarily due to solar flux variations, is much less than the trend determined from recently available satellite data. Part of this may be explained by the failure to include the effects of the Antarctic "ozone hole" in this study. However, there are also many questions remaining about the reliability of trends derived from satellite data due to questions about possible instrument drift.

Another finding of this study was that the calculated effect of the anthropogenic trace gas emissions gave a different signature in their effects on ozone with altitude and latitude than was determined for the solar cycle variations. While both the chlorofluorocarbon emissions and the ultraviolet flux variations have their primary effect on ozone in the 40–45-km region, the solar cycle variation had almost no latitudinal dependence, and the trace gases produced their maximum effect at high latitudes and had a minimum effect in the tropics. Such differences may be useful in explaining future analysis of observed trends in ozone.

These initial analyses have given a strong indication of the usefulness of the new two-dimensional model for studies of global atmospheric chemistry processes and for evaluating the impact of anthropogenic influences on the atmosphere. Future studies will extend these analyses to also study the feedback between chemical and climatic processes.

The Environmental Consequences of Nuclear War

by Joyce E. Penner, Leslie L. Edwards, Michael M. Bradley, and Steven J. Ghan

Our work on the environmental consequences of nuclear war has focused on three main areas: the effects of cloud dynamics and precipitation formation on the injection height and the microphysical scavenging of smoke above nuclear fires; the dynamical response along coastal areas to obscuring of sunlight by smoke; and the global climatic response to smoke injection. In addition, some efforts have addressed the absorption and scattering properties of smoke with branched-chain agglomerate structures.

Cloud Dynamics and Microphysics

In the event of a major nuclear war, numerous fires covering many thousands of square kilometers would be ignited. Smoke associated with these fires will be injected into the atmosphere and may cause significant near-term and perhaps even long-term climatic consequences. The extent of the impact on the climate depends critically on the amount of smoke that survives the initial cloud and precipitation that form above the fire. We are developing a set of computational tools to determine how cloud processes impact smoke plume dynamics and smoke scavenging. Our approach has been two-fold: first, to develop a detailed microphysical model capable of following the evolution of the smoke and condensed-water size distribution functions as they are affected by processes of coagulation, condensation, coalescence, break-up, and capture of aerosol by cloud drops and raindrops; second, to extend a three-dimensional cloud model to accept a high-intensity heat source, and to compute the advection of smoke and its capture by cloud and rain fields. In this latter model, the treatment of smoke and water must be parameterized: only bulk descriptions of the smoke and water fields can be computed. We plan to use the detailed microphysical model to validate the parameterizations used in the cloud/smoke plume model.

Microphysics

The primary mechanism for removing most of the submicron aerosol particles in the ambient atmosphere is nucleation scavenging. In this process aerosol particles act as the nuclei on which cloud drops form. The effectiveness of nucleation scavenging depends on the chemical and physical characteristics of the aerosol, as well as on the highest level of supersaturation that the aerosol experiences. In the ambient atmosphere and in the atmosphere above a post-attack fire, the highest supersaturation level depends on the convective updraft velocity experienced by an air parcel. This is because as an air parcel is lifted, it experiences an adiabatic expansion, as well as a mixing with air at its new altitude, which leads to a net cooling. After sufficient cooling, the air in the parcel becomes fully saturated so that condensation will start to occur. If the parcel is moving upward rapidly, the kinetics of the condensation process will be "outstripped" by the rate of cooling of the parcel. Therefore, the air in a high-velocity updraft will become more highly supersaturated than would air that is moving more slowly. An air parcel that is highly supersaturated will be able to form drops on many more aerosol particles than an air parcel that does not highly supersaturate. This is because the condensational growth equation for even very small particles can become unstable under conditions of high saturation, allowing these small particles to grow to drop size. Also, particles that have no soluble material associated with them may also form drops if high supersaturations are reached. These relationships are illustrated in Fig. 18, which shows the level of supersaturation needed to activate an aerosol particle as a function of aerosol size and mass fraction of soluble material, ϵ.

We have developed a detailed microphysics model that describes the condensational growth of water on aerosol particles of a given size distribution and chemical description (Penner and Edwards, 1986; Edwards and Penner, 1987). The model can also account for coagulation of aerosols. Also, several aerosol descriptions may be treated. Thus, a mixture of fully soluble and insoluble aerosol particles can be treated as they coagulate and mix. The model may be run alone as a box model or in conjunction with a cloud model. When run with a cloud model, the cloud model is used to specify temperature, aerosol density, and total water concentration along a trajectory, while the microphysics model is used to calculate supersaturation and water condensation on the aerosol particles.

The model has been used to explore the dependence of nucleation scavenging on updraft velocity and on the physical characteristics of the aerosol, including the mass fraction of soluble material in the aerosol, its size distribution, and the total number concentration. For example, Fig. 19 shows the fraction of aerosol mass incorporated into drops as a function of updraft velocity for an ambient concentration of aerosols with a mass fraction of $(NH_4)_2SO_4$ equal to 0, 0.01, 0.1, 0.5, and 1.0. The assumed size distribution is log normal with a mode radius of 0.05 μm and a standard geometric deviation of 2.0. As shown there, as updraft velocities increase, larger fractions of the aerosol mass are incorporated into drops. Furthermore, for the same updraft velocity, particles with a larger fraction of soluble material will be more easily scavenged. Figure 20 shows the smallest radius of particle that is scavenged for a given updraft velocity. As long as updrafts are above 5 m s^{-1}, all particles with radii larger than 0.05 microns will be scavenged. At higher updraft velocities, even smaller particles are scavenged. The nucleation scavenging mechanism is therefore able to account for the incorporation of all aerosols in the so-called "Greenfield gap" into drops. Previously, it was thought that these particles could only be scavenged via electrical processes in storms.

This model is now being used to study nucleation scavenging above nuclear-ignited fires. In such fires, mixtures of aerosols, produced from burning a variety of different materials, would be carried to cloud base. These materials would coagulate to form a complex array of chemical characteristics. The aerosol concentrations would also be much higher than those in the ambient atmosphere, leading to a lower but still substantial nucleation scavenging efficiency. Initial results imply that between 60 and 90% of the aerosol mass would enter cloud water via this mechanism.

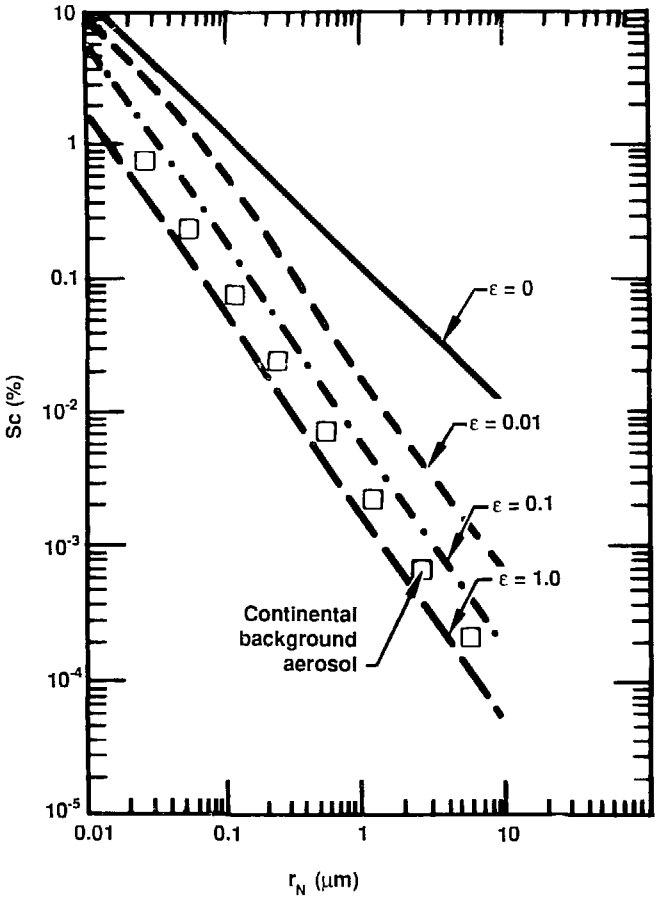

Figure 18. This figure shows the level of supersaturation needed to activate aerosol particles to grow to drops as a function of size. The aerosols are assumed to have the indicated mass fraction of $(NH_4)_2SO_4$.

Whether or not this aerosol would eventually be removed by precipitation will be the subject of future research.

Cloud and Plume Dynamics

Post-attack fires would be characteristically different from conventional, large city fires or forest fires that spread from one or a few localized points of ignition. The horizontal sizes of the individual heat and smoke sources in the post-attack fires would be much larger because the thermal energy from nuclear detonations would simultaneously ignite combustible material over large areas. The smoke plumes could rise much higher than those from conventional fires because of the intense heat from these large burning areas and the additional buoyancy that would be provided when the rising air reached the condensation level. The updrafts in these smoke plumes could reach speeds on the order of 100 m s^{-1}, and the airflow could be affected for tens of kilometers away from the

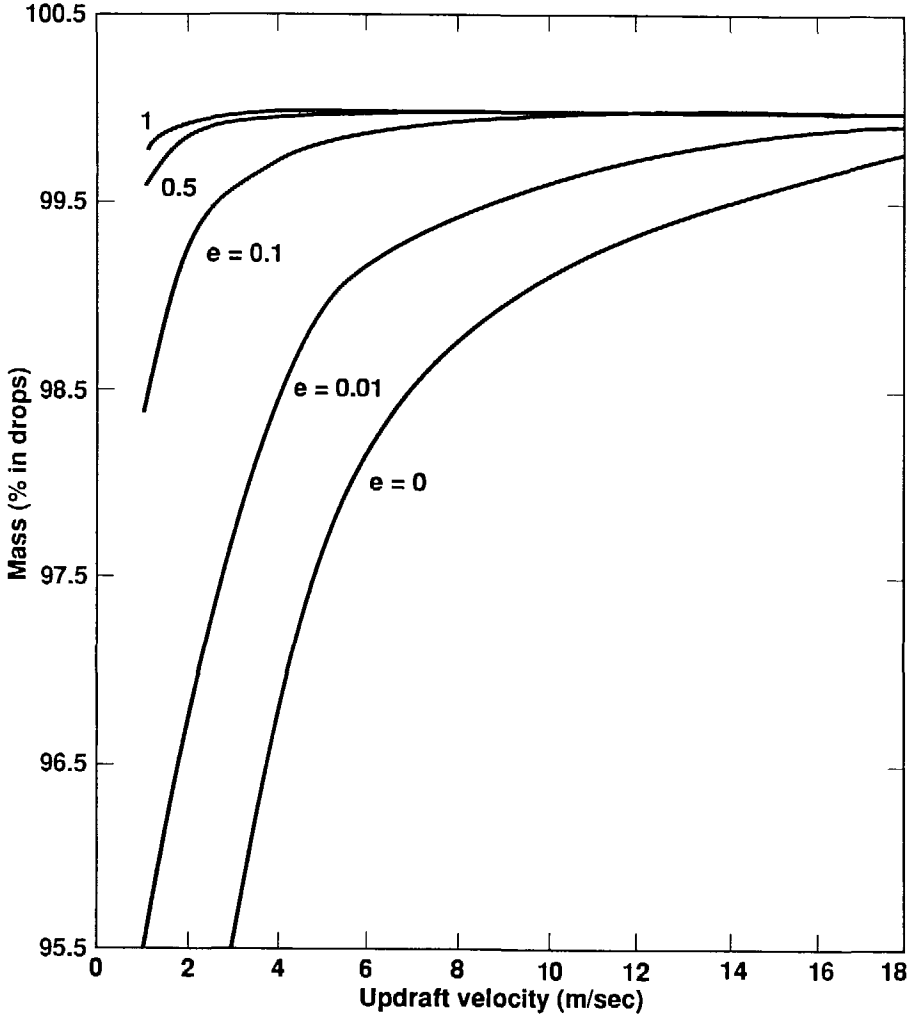

Figure 19. This figure shows the fraction of aerosol mass incorporated into drops by nucleation scavenging as a function of the updraft velocity. The aerosols are assumed to have the indicated mass fraction of $(NH_4)_2SO_4$.

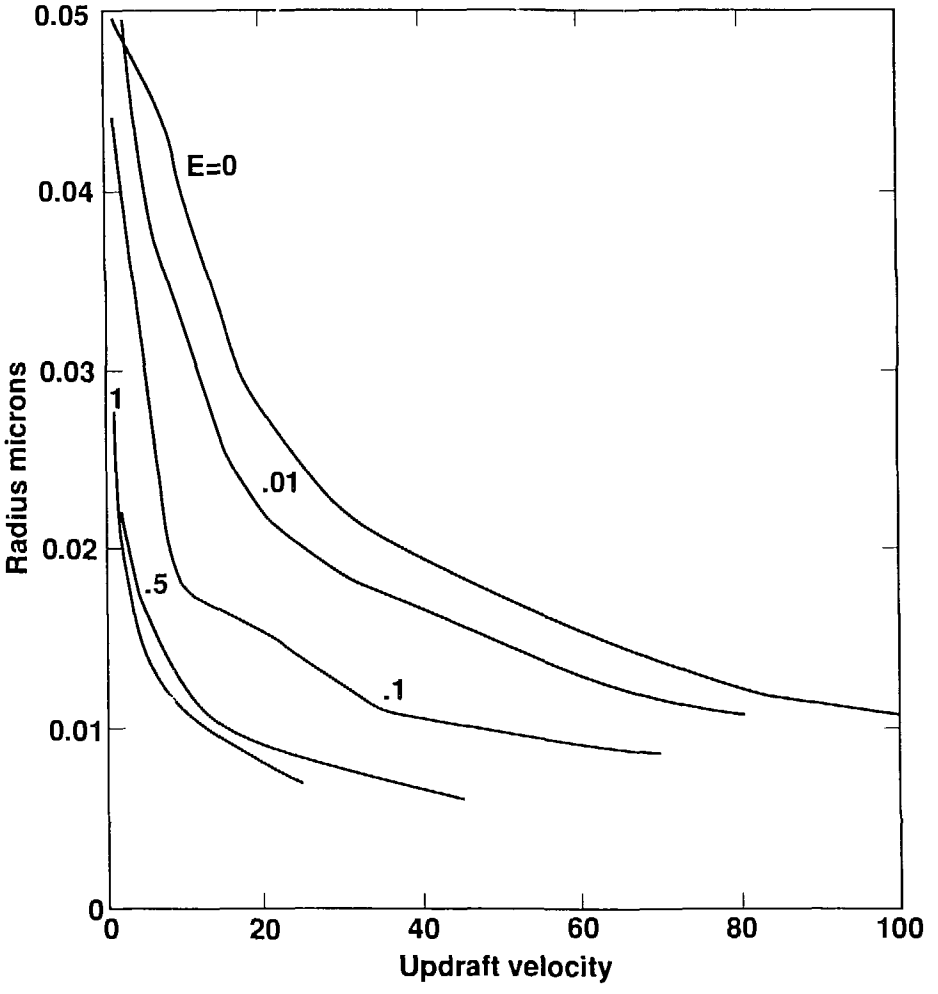

Figure 20. This figure shows the "critical radius" of particles incorporated into drops by nucleation scavenging as a function of the updraft velocity. All particles above this radius act as cloud condensation nuclei. The aerosols are assumed to have the indicated mass fraction of $(NH_4)_2SO_4$.

fires. These dynamic conditions must be properly specified in order to provide an appropriate environment for critical microphysical processes.

Although simulating these post-attack smoke plumes required the development of a new smoke plume model, it was not necessary to develop a new dynamic framework. Because of the plumes' dynamic similarity to severe convective storms, a well-known and widely accepted three-dimensional numerical cloud model was selected as the foundation for the new model. The original cloud model (Klemp and Wilhelmson, 1978) includes prognostic equations for the three velocity components, pressure, potential temperature, turbulent kinetic energy, and mixing ratios for water vapor, cloud water, and rain water. These nine equations are represented by finite-difference equations and integrated in time on a Cray supercomputer.

The Klemp-Wilhelmson cloud model was chosen as the basis for the smoke plume model because of its proven performance and computational efficiency. It has been used to simulate the airflow both inside and outside of supercells, the generation of new thunderstorm cells along outflow boundaries, the generation of new storms where two outflow boundaries collide, and the behavior of squall lines. It has also been used to study the sensitivity of dynamic development to environmental properties, such as the vertical structure of the wind, temperature, and moisture fields. Most recently, the model has been used to successfully simulate the development of a tornadic vortex.

Modeling post-attack smoke plumes requires simulation not only of natural cloud dynamics and microphysics, but also of the many possible interactions of smoke particles with water vapor, cloud droplets, raindrops, and various types of ice particles. During the initial expansion of the Klemp-Wilhelmson cloud model to a smoke plume model, three additional prognostic equations were developed to account for smoke particles and their interactions with cloud droplets and raindrops (Bradley, 1987). Figure 21 shows the results of three two-dimensional smoke plume simulations using a nucleation-scavenging parameterization based on earlier work by Molenkamp (1974). Note that the scavenging process is affected by the fire intensity and the ambient wind. Figure 22 shows a three-dimensional smoke plume for a large fire with ambient wind. Early three-dimensional simulations suggest that the sensitivity to wind speed may be artificially high in the two-dimensional simulations.

The nucleation scavenging parameterization in the smoke plume model is being upgraded so that the fraction of the smoke aerosol that is incorporated into cloud droplets will be determined using results from the detailed microphysical model of Penner and Edwards (described in the preceeding section). To adequately simulate the passage of smoke through deep, fire-driven clouds, it will be necessary to include ice processes in the model. Work on ice processes and ice-smoke interactions is currently underway, and six more equations will soon be added to the model. When this latest addition is completed, the new smoke plume model will be twice as large as its well-known parent thunderstorm model.

Chronic Effects of Large Atmospheric Smoke Injections

Recent calculations of the climatic effects of large summertime injections of smoke into the troposphere have indicated that a substantial amount of the smoke would be lofted into the stratosphere, where removal is relatively slow. For example, the smoke residence time in the atmosphere in some simulations is increased to about six months, much longer than the typical, few-week residence time of aerosols in the ambient troposphere. This suggests the possibility that processes with longer time scales than those considered in estimating acute effects may be important. Thus, interactions with sea ice, which has a time scale of months, and with the ocean mixed layer, which has a time scale of years, are likely to be important in determining any chronic effects of such large smoke injections.

To treat these feedback processes, we have applied a general circulation model of the atmosphere (Ghan et al., 1987b), coupled with models of the ocean mixed layer and sea ice, to the issue of the

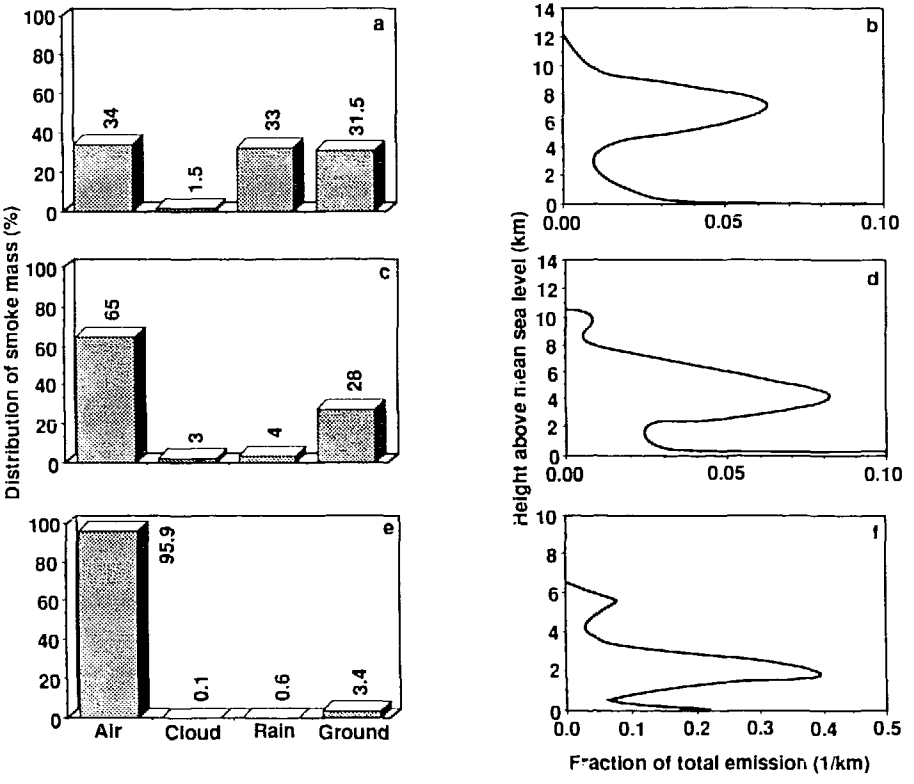

Figure 21. Distribution of smoke (interstitial, in cloud droplets, in raindrops, and deposited on ground by precipitation) shown as percent of total smoke emitted, and corresponding normalized vertical interstitial smoke profile after one hour of simulated time using $C = 100$ and Kessler autoconversion parameterization for: (a) and (b), high-intensity fire with no ambient wind; (c) and (d), high-intensity fire with ambient wind; (e) and (f), medium-intensity fire with ambient wind.

chronic climatic effects of a moderate summertime smoke injection (Ghan et al., 1987a). Except during the first 30 days following the smoke injection (in which smoke transport and removal from the troposphere are explicitly simulated), smoke amounts are prescribed in the stratosphere, with removal based on an assumed six-month half-life. Smoke in the stratosphere is assumed to be spread uniformly over the globe; such rapid dispersal is a consequence of the acute phase modification of atmospheric circulation.

The longitudinal and monthly average land-surface temperature and ocean-mixed-layer temperature changes resulting from the smoke are illustrated as functions of latitude and time in Fig. 23. Within the first few months following the smoke injection, maximum cooling of the ocean mixed layer is predicted to be about 4° C in midlatitudes, with expanded sea ice coverage in arctic regions. The increased sea ice coverage reduces the effective heat capacity of the ocean surface,

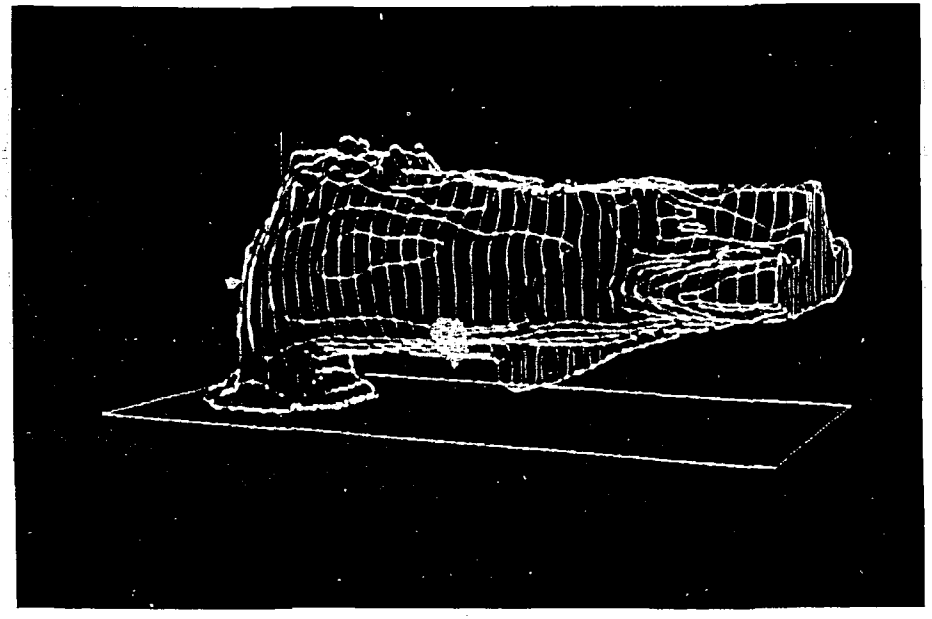

Figure 22. Forty minutes after ignition, the smoke plume from an intense fire rises 13 km above Earth's surface and extends more than 40 km downwind.

leading to a colder winter in oceanic regions with expanded sea ice. Southern Hemisphere land surfaces cool by about two degrees during the following southern summer as a direct result of the smoke-induced reduction in insolation. The following northern summer is found to be two degrees cooler in Northern Hemisphere midlatitude continental regions, partly because of the reduced insolation and partly because of the long memory of the oceanic component of the climate system.

Surprisingly, we find that the ocean mixed layer deepens considerably in some regions in response to the smoke injection. For example, during the first 30 days, the ocean mixed layer in the tropical eastern Pacific deepens some 80 m (to about double its normal depth) as a result of the combination of an eastward sloshing of the mixed layer driven by a shift in surface wind patterns, and increased entrainment of deep ocean water due to both surface cooling and enhanced mechanical stirring associated with the shift in wind patterns. This response is in some respects similar to the El Niño phenomenon, which occurs periodically in the tropical east Pacific.

In the future we plan to repeat the above experiment using a larger initial smoke injection, and to apply a general circulation model with finer vertical resolution to determine whether the shifted wind patterns simulated by our tropospheric general circulation model would indeed be a feature of the atmospheric response.

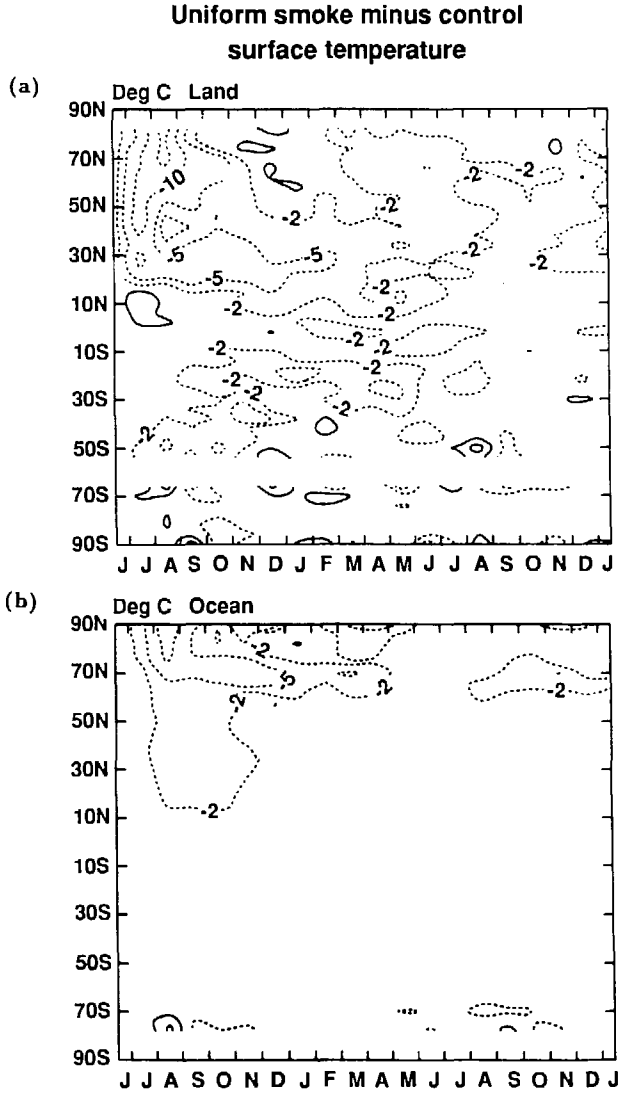

Figure 23. The smoke-induced change in surface temperature averaged over land (a) and ocean (b) grid points as a function of latitute and time, from July (time of smoke injection) to January of the second year. Contour levels are $\pm 2°$ C, $\pm 5°$ C, $\pm 10°$ C, and $\pm 15°$ C. Changes not persisting longer than one month, such as appear near the south pole, are not considered physically significant.

Modeling the Czochralski Growth of Oxide Crystals

by Jeffrey J. Derby and Philip M. Gresho

The availability of large, single-oxide crystals of materials such as Nd:YAG (neodymium: yttrium aluminum garnet) is important for the further development of solid-state lasers in the inertial confinement fusion and defense programs. To meet the optical requirements for a laser material, these crystals must be relatively free from defects and internal strain, and their macroscopic properties, such as dopant distribution (neodymium in the above-mentioned case), need to be nearly homogeneous. The production of such crystals large enough to adequately serve the needs of the Laser Program is an ambitious undertaking. Although manufacturers of electronic devices have been relatively successful in developing techniques that enable the growth of large (greater than 6-in.-diameter), defect-free silicon crystals, the analogous scale-up of oxide crystal growth processes has been far less successful. There are numerous reasons for this lack of progress; however, a major factor is the lack of a fundamental understanding of the transport of heat and mass, which control the Czochralski (CZ) growth process. In this process, the large single crystals are "pulled" from a melt comprising a fluid mechanical system of oxides, dopants, and impurities.

The growth of large oxide crystals of high quality is technically demanding, because precise control of a multiphase system that includes molten oxides must be maintained for long periods of time (days to weeks) at very high temperatures (usually 2000–2300 K). Owing to these challenges, crystal growth technology has progressed (evolved) rather slowly and the field is often viewed by its practitioners as equal parts of art and science. As such, incremental advances in technology are usually guided by past experience, empiricism, intuition, and luck. Empirical evidence has shown that the existing knowledge, based on small-scale CZ oxide growth, is insufficient to rapidly advance current practice to that required for the growth of large-dimension oxide crystals. There is thus a need to accelerate process development through a rational approach that is based on a fundamental assessment of the relevant issues. The knowledge gained through modeling will greatly aid this effort.

The goal of the CZ modeling project at LLNL is to quantitatively model the CZ growth of oxide crystals and establish a scientific basis for understanding the process. This is being accomplished with the aid of sophisticated numerical models based on the finite-element method, which account for both the highly nonlinear interactions among field quantities, such as temperature, velocity, and solute concentration, and the system interfaces, such as the solidification front between melt and crystal, the melt meniscus, and the shape of the growing crystal (Derby et al., 1988). This model is coupled with one that provides an analysis of induction heating to link the events in the melt and crystal to growth conditions set by the process operator (Gresho, 1987; Gresho and Derby, 1987a; Gresho and Derby, 1987b; Derby and Atherton, 1988).

Figures 24–26 show schematic descriptions of the physical system being studied and a sample of some interesting recent results.

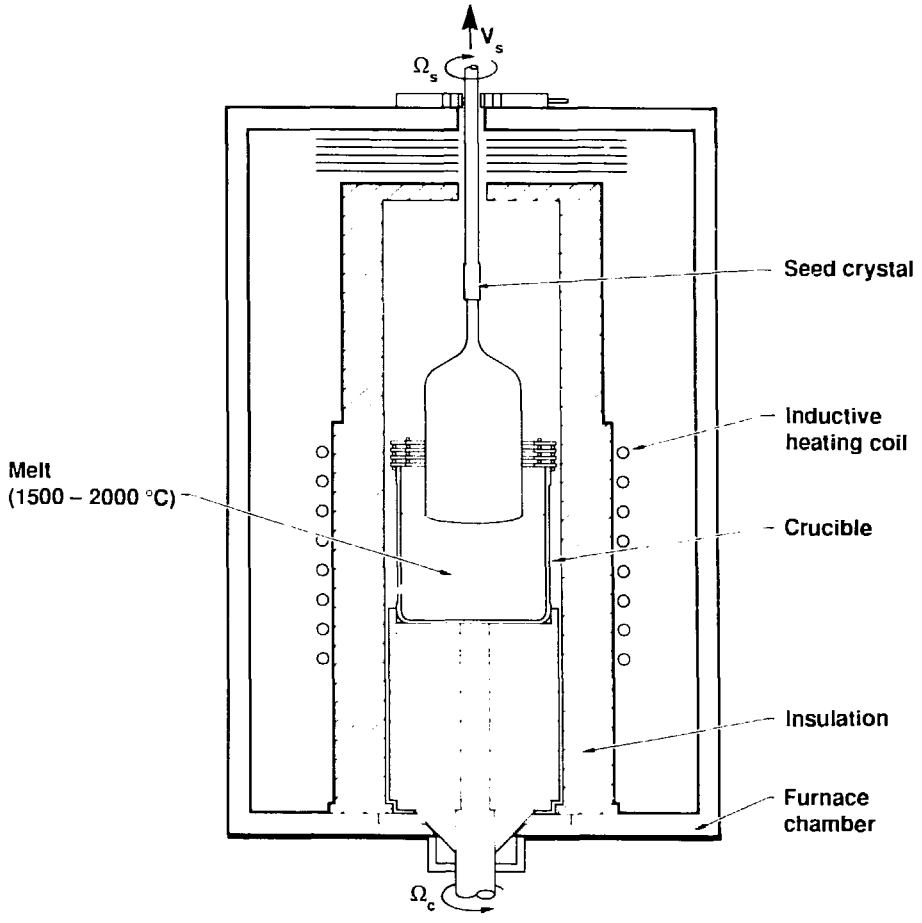

Figure 24. Schematic diagram of the Czochralski method of growing a single crystal from its melt. Process conditions are determined largely by overall heat transfer in the system and fluid mechanics in the melt.

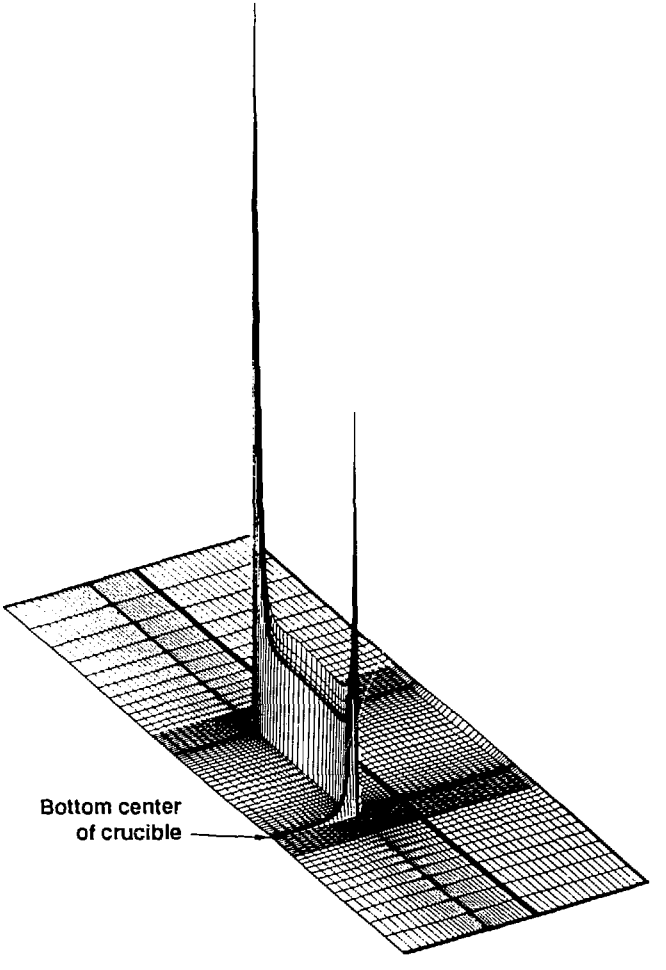

Figure 25. Perspective plot of the rate of heat generation in the crucible, produced by the inductive heating system. Power is deposited primarily in the outer wall with local maxima located near the upper lip and bottom corner of the crucible.

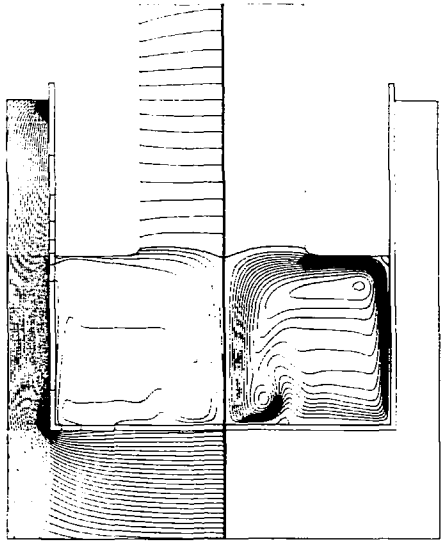

Figure 26. Finite-element model predictions of the temperature field and the melt hydrodynamics for the Czochralski growth of Gadolinium Gallium Garnet. The vertical line at the center of the figure corresponds to the axis of the system. The left half of the plot shows temperature contours in the crystal, melt, crucible, and the insulation and pedestal that surround the crucible; heat flows predominantly from the hot crucible wall through the melt and upward into the crystal. The right figure half presents streamlines of the flow field in the melt; the primary recirculation cell rotates counter-clockwise with warm fluid rising along the crucible wall and cooler fluid falling along the melt centerline.

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Appendix A. Division Scientists and Supporting Staff

G-Division Scientific Staff

Name	Research Interests	Degree	School
Cynthia S. Atherton	*atmospheric chemistry*	M.S.	Massachusetts Institute of Technology
Michael M. Bradley	*cloud dynamics, microphysics*	Ph.D.	U. Illinois
Stevens T. Chan	*atmospheric dynamics*	Ph.D.	U. of Calif., Davis
Peter S. Connell	*photochemical kinetics*	Ph.D.	U. of Calif., Berkeley
Curtis C. Covey	*fluid-dynamical simulation*	Ph.D.	U. of Calif., Los Angeles
Jeffrey J. Derby	*numerical (finite-element) methods in transport processes*	Ph.D.	Massachusetts Institute of Technology
Marvin H. Dickerson	*real-time dose modeling, model evaluation*	Ph.D.	Florida State U.
Leslie L. Edwards	*numerical modeling; atmospheric microphysics, hydrodynamics*	M.A.	U. Oregon
James S. Ellis	*remote sensing of climatic change*	Ph.D.	Colorado State U.
Hugh W. Ellsaesser (retired, participating guest)	*atmospheric dynamics, climate change*	Ph.D.	U. Chicago
Donald L. Ermak	*turbulence, atmospheric heavy-gas dispersion*	Ph.D.	U. of Calif., Davis
Kevin T. Foster	*boundary layer meteorology*	M.S.	U. of Calif., Davis
Steven J. Ghan	*climate dynamics*	Ph.D.	Massachusetts Institute of Technology
Keith E. Grant	*radiation transport, uncertainty analysis, transport-kinetics models*	Ph.D.	U. of Calif., Davis/Livermore
George D. Greenly, Jr.	*planetary boundary layer meteorology*	M.S.	U. Oklahoma
Philip M. Gresho	*computational fluid mechanics, numerical methods*	Ph.D.	U. Illinois
Stanley L. Grotch	*data analysis*	Ph.D.	Massachusetts Institute of Technology
Paul H. Gudiksen	*radiological impact studies, meteorological measurements*	Ph.D.	U. Washington
Ted F. Harvey	*aerosol science, environmental radiation, source terms*	Ph.D.	U. of Calif., Davis
Douglas E. Kinnison	*trace-gas chemistry interactions*	Grad.Student	U. of Calif., Berkeley
Ronald P. Koopman	*heavy-gas dispersion, accidental release of toxics*	Ph.D.	U. of Calif., Davis/Livermore
Kenneth C. Lamson	*health physics, field measurement systems*	M.S.	U. Pittsburgh
Rolf Lange	*turbulence and diffusion*	Ph.D.	U. of Calif., Davis
Robert L. Lee	*planetary boundary layer modeling*	Ph.D.	U. of Calif., San Diego
John M. Leone, Jr.	*atmospheric numerical modeling*	Ph.D.	Iowa State U.
Michael C. MacCracken	*global climate studies*	Ph.D.	U. of Calif., Davis/Livermore
John W. McClure	*physics*	B.S.	U. Southern California
Connee S. Mitchell	*boundary layer meteorology*	M.S.	Oregon State U.
Charles R. Molenkamp	*cloud microphysics, mesoscale modeling, cloud modeling*	Ph.D.	U. Arizona

Joyce E. Penner	*microphysics and atmospheric chemistry*	Ph.D.	Harvard U.
Kendall R. Peterson	*atmospheric diffusion*	M.S.	U. Chicago
Gerald L. Potter	*climate change and model sensitivity studies*	Ph.D.	U. of Calif., Los Angeles
Howard C. Rodean	*turbulence, material phase change*	M.S.	Purdue U. and Southern Methodist U.
Daniel J. Rodriguez	*model evaluation and boundary layer studies*	M.S.	Calif. State U. San Jose
Leonard C. Rosen	*atmospheric optics and wave propagation*	Ph.D.	Columbia U.
Thomas J. Sullivan	*mesoscale meteorology, air pollution, emergency assessment*	Ph.D.	U. of Calif., Davis
Karl E. Taylor	*climate dynamics, atmospheric dynamics*	Ph.D.	Yale U.
John J. Walton	*modeling and code development, global transport and dispersion*	Ph.D.	U. Kansas
Donald J. Wuebbles	*atmospheric chemistry, chemical-climate interactions, numerical modeling*	Ph.D.	U. of Calif., Davis

G-Division Supporting Staff

Name	Position
Julia J. Bagorio	Secretary
Marilyn B. Borton	Secretary
Pamela M. Drumtra	Division Secretary
K. Patrick Ellis	Field Support
Doris G. Gresho	Secretary
Nancy A. Kliment	Secretary
Mabel K. Moore	Secretary
Lonnette L. Robinson	Secretary
Charles R. Veith	ARAC Facilities Coordinator
Floy L. Worden	Resource Manager

Affiliated Staff

Name	Affiliation	Discipline	Degree	School
Rosemary O. Abriam	1	*computer science, biology*	B.S.	Calif. State U., Hayward
Ronald L. Baskett	3	*atmospheric sciences*	M.S.	U. of Calif., Davis
Richard D. Belles	1	*applied science*	M.S.	U. of Calif., Davis
Diane F. Bonner	1	*mathematics*	B.S.	State U. of N.Y., Albany
Sharon C. Braley	1	*general education*	A.A.	Chabot College
Thomas C. Brown	2	*applied science*	M.S.	U. of Calif., Davis
Stephen P. Cooper	1	*computer science*	B.S.	Purdue U.
DeeAnn R. Davi	3	*mathematics*	B.A.	Westmont College
Harold E. Eddleman	1	*electronic engineering*	B.S.	U.S. Naval Postgraduate School, San Diego
Robert P. Freis	1	*engineering science*	M.S.	U. of Calif., Berkeley

Yolanda Y. Gagaza	3	*general education*	A.A.	Ohlone College
Donald A. Garka	2	*electronics engineering*	B.S.	Devry Inst. Tech.
Glenn L. Hage	1	*mathematics*	B.A.	San Jose State U.
Anthony T. Hoang	3	*computer science*		San Jose State U.
John K. Hobson	1	*mathematics*	M.S.	U. of Calif., Berkeley
Leonard A. Lawson	1	*mathematics*	A.B.	Calif. State U., Chico
Ambrosio R. Licuanan	1	*computer science*	A.A.	Ohlone College
Gloria L. Martin	3	*computer science*		Chabot College
Mary A. Mansigh	1	*mathematics, chemistry*	B.S.	U. Miami
Louise K. Morris	1	*mathematics*	B.S.	U. of Calif., Davis
John S. Nasstrom	3	*atmospheric sciences*	M.S.	U. of Calif., Davis
Charles J. O'Connor	1	*computer science*	M.S.	Calif. State U., Hayward
Walter W. Schalk, III	3	*meteorology*	M.S.	Florida State U.
E. Eugene Schultz, Jr.	2	*experimental psychology*	Ph.D.	Purdue U.
Denise A. Sumikawa	1	*computer science*	M.S.	U. of Calif., Davis
Raymond L. Tarp	1	*mathematics*	B.A.	San Jose State U.
Sandra S. Taylor	1	*computer science*	B.S.	Iowa State U.
Hoyt Walker	1	*computer science*	M.S.	U. of Calif., Davis
Jon G. Welch	2	*electronic technology*		
Conrad A. Wilgus	1	*applied mathematics*	M.S.	Calif. State U., Sacramento
Dean N. Williams	1	*computer science*	M.S.	Calif. State U., Chico
Carolyn D. Wimple	1	*computer science*	B.S.	Calif. State U., Sacramento

1. Computations Department (LLNL)
2. Engineering Department (LLNL)
3. EG&G

Consultants*

Name	Discipline	Organization
James F. Barbieri	*database management*	U.S. Navy
Joseph B. Knox	*interactions of energy and climate, modeling of transport and diffusion of pollutants on spatial scales*	LLNL, (Retired), Assistant to the Associate Director for Physics
Richard C. Orphan	*resource management*	Private
John L. Stout	*geology*	KMI Associates
Ronald D. Tilden	*creativity enhancement*	Tilden & Associates

* Names (and projects) of those consultants involved with the Division on a continuing basis are found in Appendix B.

Appendix B. LLNL–University Interactions by Project

DOE

OHER—Regional Modeling

U. of Colorado (Robert L. Sani), *fluid mechanics, applied mathematics*

BES—Clouds/Radiation

U. of Maryland (Robert G. Ellingson), *modeling atmospheric radiation*

BES—Climate Program Management

Ocean Research Consultants (U. of Calif., San Diego), *detection of climate change*

U. of East Anglia (T. M. L. Wigley), *intercomparison of simplified ocean models*

BES—Trace Gases

U. of Calif., Berkeley (Douglas E. Kinnison, graduate student), *trace gas-chemistry interactions*

BES—Model Comparison

State U. of New York (SUNY)/Stony Brook (Robert D. Cess), *climatic effects of arctic aerosols, GCM intercomparison*

Oregon State U. (W. Lawrence Gates), *global climate modeling*

OHER—ASCOT Modeling

Pennsylvania State U. (Alfred K. Blackadar), *boundary layer modeling over complex terrain*

U. of Calif., Los Angeles (Morton G. Wurtele), *boundary layer meteorology*

OMA—Global Effects

Desert Research Institute, U. of Nevada (John Hallett), *microphysics and scavenging*

U. of Calif., Los Angeles (Steven K. Krueger), *turbulence*

U. of Illinois (Robert B. Wilhelmson), *three-dimensional cloud modeling and cloud physics*

National Center for Atmospheric Research (Joseph B. Klemp), *meteorology, computer science*

U. of Utah (Magdy Iskandar), *radiative effects of nonspherical particles*

G-Division

U. of Maryland (Robert G. Ellingson), *radiation transport*

Reimbursable/Work for Others

DOD

DNA—Environmental Consequences

Desert Research Institute, U. of Nevada (John Hallett), *microphysics*

DNA—Deposition

San Francisco State U. (Charles S. Shapiro), *radiological impact of large scale releases of nuclear material*

U. of Florida (Arthur A. Broyles), *human survivability from acute gamma radiation exposure*

GBL—Atmospheric Propagation

U. of Florida (James Ipser), *laser propagation processes*

NASA

UARS

State U. of New York, Albany (Julius Chang), *satellite-model data comparisons*

LLNL

Richard Eckman (Post Doc starting in 1988), *global modeling of aeronomy processes*

Gas Research Institute/DOT

Colorado State U. (Robert Meroney), *wind tunnel modeling of LNG vapor fence experiments*

U. of Arkansas (Jerry Havens), *FEM3 modeling of LNG vapor fence experiments*

Appendix C. Special Outside Staff Activities

Michael M. Bradley: *Co-chairman for Cloud Physics, Interagency Lightning Threat Warning Working Group*

Peter S. Connell: *Member, National Aeronautics and Space Administration/Chemical Manufacturers Association (NASA/CMA) Experts "Tiger" Team on Ozone and Temperature Trends*

Curtis C. Covey: *Thesis advisor for three students at the U. of Miami and one student at Pennsylvania State U.*

Marvin H. Dickerson: *Member of the DOE Subcommittee on Dose Assessment; Consultant for the International Atomic Energy Agency in the area of emergency preparedness*

George D. Greenly, Jr.: *Vice chairman, Basic Sciences and Technology Division of the Air Pollution Control Association (APCA); Member of TT-3 Meteorology Committee of APCA; American Meteorological Society Certified Consulting Meteorologist (CCM)*

Philip M. Gresho: *Editor, International Journal for Numerical Methods in Fluids; Member of editorial board, Communications in Applied Numerical Methods; Member of editorial board, Latin American Journal of Heat and Mass Transfer*

Joseph B. Knox: *Bluenose Panel Member; LLNL Representative to Lawrence Berkeley Laboratory for Environmental Policy Center; LLNL Representative to DOE-OHER Global Effects Research Committee*

Ronald P. Koopman: *Scientific Advisor, DOE/Nevada, Liquefied Gaseous Fuels Spill Test Facility*

Robert L. Lee: *Member of editorial board, International Journal for Numerical Methods in Fluids*

Michael C. MacCracken: *Principal Scientist for Climate of DOE CO_2 Research Program; U.S. Co-Chair of Climate Project of U.S.-U.S.S.R. Working Group VIII; Chairman, NAPAP Regional Acid Deposition Model review committee; Co-author WMO/ICSU Joint Scientific Committee report on nuclear winter research; Associate Editor, Journal of Climate*

Joyce E. Penner: *Defense Nuclear Agency Field Experiment Planning Committee*

Thomas J. Sullivan: *Emergency response team leader (ARAC); accident response team member (ARG); terrorist response team member (NEST)*

Karl E. Taylor: *Associate Editor, Journal of Geophysical Research*

Donald J. Wuebbles: *Member, NASA-WMO Panel on Modeling of Trace Gas Effects; Member, NASA/CMA Experts "Tiger" Team on Ozone and Temperature Trends; U.S. Representative at UNEP and other international meetings concerning potential impacts of trace gases on ozone; thesis advisor for student from U. of Calif., Berkeley*

Appendix D. 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, subdivided into five categories that describe their primary application. The scientists currently having primary responsibility for each code are also listed; these individuals are not necessarily the developers of the model.

Species Transport and Diffusion Models

MATHEW/ADPIC Model

This three-dimensional particle-in-cell (PIC) model (ADPIC) calculates the transport and diffusion of a puff or plume in a time-varying atmospheric boundary layer. 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. 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. ADPIC calculations have been compared against measurements for many field-diffusion experiments, including the ASCOT program and for emergency and assessment response, such as the 1979 TMI incident, the subsequent Presidential Commission investigation, and the 1986 Chernobyl accident. A new version of the model, suitable for studying long-range transport and chemistry of several days, is currently being developed.

Contact: Rolf Lange

HMEDIC/HADPIC

HADPIC is a version of ADPIC modified to provide a capability to model transport and diffusion of pollutant clouds in the troposphere of the Northern Hemisphere using three-dimensional wind fields. These wind fields are constructed in the ARAC central facility from Air Force Global Weather Central gridded wind data. HMEDIC is a data-handling and interpolation code that processes the AFGWC gridded data, either analysis or forecast, into three-dimensional arrays. HADPIC provides as output the pollutant concentrations at selected regions over the Northern Hemisphere. The code was used to simulate the time and space evolution of the 1986 Chernobyl reactor accident.

Contact: Rolf Lange, Thomas J. Sullivan, Robert P. Freis

GRANTOUR Model

GRANTOUR is a global atmospheric model that uses prescribed winds to transport species using a Lagrangian-sampler-parcel approach to calculate advection of tracers very accurately. The model can also calculate, if appropriate, scavenging (given precipitation rates), coagulation, chemistry, 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 and LLNL/Community Climate Model). The model has also been used to study the global distribution of HNO_3 resulting from NO_x sources, chemistry, and precipitation scavenging.

Contact: John J. Walton

Advection-Diffusion FEM Model

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

Contact: Philip M. Gresho, Robert L. Lee

Tracer Trajectory Model

This model uses data on 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 trajectories may be followed for (1) constant height above terrain, (2) constant parcel potential temperature, or (3) constant parcel pressure. Dispersal of the tracer by eddy mixing (or diffusion) is not considered.

Contact: Ronald L. Baskett

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. The diffusion coefficients can be time-dependent. An Eulerian grid at Earth's surface keeps track of the cloud's position and provides the framework for calculating air concentrations during its passage. A conversational version of 2BPUFF is on ARAC's computer system.

Contact: Kendall R. Peterson

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 multiline input mode, the user specifies whether the release is routine or accidental. The output consists of both average concentration and deposition contours, and contours for various probabilities that specific values will be exceeded.

Contact: Kendall R. Peterson

Radionuclide Models

CAP Model

The Containment Atmosphere Physics (CAP) model capability simulates reactor-containment building scavenging processes. To be flexible and process-oriented, this simulation is based on methods of systems dynamics; i.e., if new physical processes seem 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 database and a simulation that realistically describes the scavenging processes inside a containment building when its equation of state is driven by gaseous releases from a melting core.

Contact: Ted F.Harvey, Leslie L. Edwards

KDFOC2 Model

This versatile fallout model 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 and other databases available in G-Division provide the essential tools for considering tradeoffs between various plans and features of different nuclear scenarios and for estimating the technical uncertainties inherent in the predictions.

Contact: Ted F. Harvey

GLODEP2 Model

The GLODEP2 model provides estimates of the surface deposition of worldwide radioactivity and the gamma-ray dose-to-man from intermediate and long-term fallout produced by nuclear explosions. The model is based on empirical relationships derived primarily from injection-deposition experience gained from the U.S. and the U.S.S.R. nuclear tests in 1958. If a nuclear power facility is destroyed (vaporized) and its debris behaves in the same manner as the radioactive cloud produced by the nuclear weapon that attacked the facility, the model can predict the gamma dose from this source of radioactivity. Empirically derived gamma dose relationships 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, and results compare well with observations.

Contact: Leslie L. Edwards, Ted F. Harvey, Kendall R. Peterson

MISER Model

The MISER model treats 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 nuclide transport. The results of the ORIGEN and BIODOSE codes are used to determine 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 eight 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.

Contact: Ted F. Harvey, Leslie L. Edwards

Atmospheric Chemistry, Radiation, and Microphysics Models

One-Dimensional Chemical-Radiative-Transport Model

The one-dimensional model calculates (globally) averaged, vertical profiles of relevant trace gas concentrations in the troposphere and stratosphere. This model is a useful diagnostic and prognostic tool for studying chemical, radiative, and dynamical processes and interactions in the atmosphere. It has been used extensively for national and international investigations of the effects of potential chemical emission scenarios upon the ozone layer. Modes of model execution include diurnally cycled or diurnally averaged, for time-dependent scenarios or rapidly obtained steady-state solutions. The model atmosphere extends from the ground to just above the stratopause (approximately 56 km) and is divided into 44 layers. The model chemistry includes approximately 130 chemical reactions among 40 species. The radiative treatment for photolysis reactions includes the effects of multiple scattering. Changes in radiatively active trace-gas concentration can be used to obtain new stratospheric-radiative-equilibrium temperatures. Transport processes in the one-dimensional model are simulated by prescribed diffusion coefficients.

Contact: Donald J. Wuebbles, Peter S. Connell, Keith E. Grant

Two-Dimensional Chemical-Radiative-Transport Model

The two-dimensional model calculates the zonally averaged, time-dependent concentrations of relevant tropospheric and stratospheric trace gases as they vary with latitude, altitude, and season. This model currently uses a grid with 16 latitude zones and 18 vertical layers. It includes approximately 100 reactions among thirty species, including 27 photolysis reactions. Diabatic winds are calculated using model-derived-radiative and latent-heating rates, assuming prescribed seasonally varying initial temperatures. These prescribed temperatures are appropriate for ambient trace-gas concentrations. For chemical perturbation scenarios, either temperatures or diabatic winds can be varied as radiatively active trace species are perturbed from their ambient concentrations.

Contact: Donald J. Wuebbles, Peter S. Connell, Keith E. Grant

Multi-Layer Air Quality Model

This Eulerian code was developed to describe the long-range, multi-day transport and chemical interactions of air pollutants in which pollutants may be isolated overnight in an elevated layer and reincorporated 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 in order to preserve 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 is used to describe the transport above the mixed layer; 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 specified 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 has recently been applied to study the coupling of the Monterey and Bay Area air basins.

Contact: Joyce E. Penner, Peter S. Connell

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, photochemical kinetics, and surface deposition. It requires specification of 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 or preprocessor for each major calculational step, including 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. 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 have been applied to studies in the San Francisco Bay Area and around St. Louis, Missouri.

Contact: Joyce E. Penner, Peter S. Connell

Atmospheric Kinetics Model

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

Contact: Donald J. Wuebbles, Joyce E. Penner, Peter S. Connell

CAMP Model

The CAMP computer code numerically solves the atmospheric microphysical equations in a well-mixed spherical or plume-like parcel of air, water vapor, liquid water, and aerosols. The aerosols may be of differing compositions of water-soluble and insoluble materials. The parcel may be pseudo-adiabatic, where the dynamics are driven by the buoyancy forces acting on a background sounding, or based on a specified "trajectory," for which the dynamics are determined by a cloud-scale dynamics code. The parcel may entrain background aerosols and drops. Given an aerosol-number density distribution and/or a drop-number density distribution, the code solves for the time evolution of the distributions as well as for the parcel temperature and saturation. The microphysical processes included are: condensation/evaporation of water vapor, nucleation of drops, aerosol coagulation, drop coalescence, interstitial aerosol collection by drops, and drop break-up—all on spherical particles. The model does not yet consider electrical effects or ice processes, both of which may be important in some applications.

Contact: Leslie L. Edwards, Joyce E. Penner

Aerosol Coagulation Model

This model solves the kinetic coagulation equation, which determines the evolving size distribution of an assemblage 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 specified from observations or calculation. A submodel is available 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. It is currently being revised to consider several vertical layers to explicitly account for vertical diffusion and aerosol sedimentation.

Contact: Joyce E. Penner

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's Cumulus Dynamics Model, 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 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.

Contact: Charles R. Molenkamp

STRATSCAV Model

This model is based on a module used in 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, implying that a one-dimensional cloud model can be used to derive the vertical distribution of clouds, rain, and snow. These hydrometeors then interact with the pollutant particles to scavenge, redistribute, and deposit them. A surface-based grid gives the horizontal distribution of the removed pollutant.

Contact: Charles R. Molenkamp

RAD1 Solar Radiation Model

This model solves the radiative transfer equation for a cloudless, plane-parallel atmosphere using a successive-scattering iterative procedure. It 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. The model was originally developed in the early 1970s by J. V. Dave of International Business Machines (IBM).

Contact: Keith E. Grant

SWPAK

This model computes upward and downward ultraviolet and visible radiation fluxes given atmospheric vertical profiles of pressure, temperature, and concentrations of O_2, O_3, and NO_2. The calculated fluxes can be used by chemical-radiative-transport models to calculate layer heating rates or, with additional driver routines, photodissociation rates. The formulation of this model accounts for multiple scattering and allows inclusion of clouds and aerosols as well as absorbing gases. The solar spectrum and pertinent absorption cross sections are divided into 148 wavelength bins between 133.75 and 730 nm. Advantage is taken of each wavelength bin constituting an independent radiation transfer problem to allow the coding to vectorize over wavelength bins when compiled on the Cray-1 or Cray-XMP. For each plane-parallel vertical layer, the scattering and absorption of diffuse incident radiation is treated using the Sagan and Pollack two-stream algorithm. Scattering and absorption from the direct solar beam is treated using the delta-Eddington approximation. The effects of the separate layers are combined using the adding technique.

Contact: Keith E. Grant

Hydrodynamics Models

FEM3 and FEM3A Dense-Gas-Dispersion Models

These codes have been developed primarily to simulate the atmospheric dispersion of heavier-than-air gas and liquid releases. A modified Galerkin finite-element method was employed to solve the time-dependent conservation equations of mass, momentum, energy, and species of the dispersed material together with the ideal gas law for the density of the mixture. A generalized anelastic approximation was invoked to preclude sound waves and yet allow large-density variations in space and time. Turbulence is parameterized via a K-theory submodel, and heat transfer from the ground surface into the vapor cloud is also accounted for. Both codes can solve two- and three-dimensional problems, including treatment of variable terrain and finite-duration/continuous releases. In FEM3A, instantaneous sources and obstructions are also treated. In addition, a phase-change submodel is available for handling the phase transitions (between vapor and droplets) of the dispersed material.

Contact: Stevens T. Chan, Philip M. Gresho

FEM Nonhydrostatic 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.

Contact: John M. Leone, Jr., Robert L. Lee

FEM Hydrostatic Mesoscale Model

This newest of the finite-element-based models is a spinoff from all of the earlier ones. It has been designed to provide a new capability in which both two- and three-dimensional computations over reasonably complex terrain can be performed in much less central processing unit (CPU) time than with the earlier models. This is done by solving a simpler and more restrictive set of model

equations in which hydrostatic equilibrium is assumed to exist. A version of this new model will be designed to operate on the ARAC computer system (VAX) and to thus assist in emergency response by providing actual forecast winds. A research version will be used in a simulation mode and will be continuously upgraded in its physical and mathematical capabilities.

Contact: John M. Leone, Jr., Stevens T. Chan

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.

Contact: Charles R. Molenkamp

OCTET: Dynamical and Microphysical Plume, Storm, and Mesoscale Numerical Simulation System

The OCTET Simulation System consists of eight numerical models that are applicable to a large number of atmospheric phenomena and spatial scales, ranging from dry mesoscale circulations, to tornadoes, to the interactions of aerosols with liquid and frozen precipitation inside violent, strongly electrified thunderstorms. The OCTET system uses the nonhydrostatic, compressible, three-dimensional dynamic framework of the Klemp-Wilhelmson storm model. The system has a modular structure, and new modeling capabilities are continuously being added. The simplest model in the OCTET system has only six prognostic variables; the most complex model has over twenty prognostic variables. The eight models in the OCTET system are capable of simulating the nonhydrostatic and hydrostatic dynamics and the microphysical processes in:

(1) Dry mesoscale circulations;
(2) "Warm," precipitating, convective and stratiform clouds; and warm, moist, mesoscale circulations;
(3) "Cold," ice-bearing (ice crystals, snow, graupel, and hail), convective and stratiform clouds; and severe storm circulations including squall lines, gust fronts, microbursts, low-level wind shears, and tornadoes;
(4) Lightning generation in severe, electrified storms and storm complexes (projected capability, not operational in 1988);
(5) Dry smoke plumes (e.g., from forest fires or from burning cities in post-nuclear-exchange environments); and aerosol transport and diffusion in dry mesoscale circulations;
(6) Smoke plumes in warm, moist atmospheres with condensation, liquid precipitation, and smoke scavenging and removal; and aerosol transport, diffusion, and hydrometeor-aerosol interactions in warm, moist, mesoscale circulations;
(7) Smoke plumes in cold, moist atmospheres with condensation, freezing, liquid and solid precipitation, and smoke scavenging and removal; and aerosol transport, diffusion, and hydrometeor-aerosol interactions in cold, moist, mesoscale circulations;

(8) Electrified smoke plumes; large, intense smoke plumes that interact with fire-forced, electrified, ice-bearing clouds; and aerosol transport, diffusion, and hydrometeor-aerosol and aerosol-aerosol interactions in mesoscale circulations in electrified atmospheres (projected capability, not operational in 1988).

The OCTET system is operational on the Cray-1, Cray-2, and Cray X-MP computers using both the CFT and CIVIC compilers.

Contact: Michael M. Bradley

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, but differs from their 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.

Contact: Michael M. Bradley

SLAB Dense-Gas-Dispersion Model

This code was designed to treat the atmospheric dispersion of a denser-than-air vapor release under steady-state conditions, but is also available in a finite-duration or puff version. SLAB solves the crosswind-averaged conservation equations of mass, species momentum, and energy, along with a cloud-width equation and the equation of state, using the Runge-Kutta method. The code is one-dimensional with downwind distance being the independent variable; however, the full three-dimensional concentration distribution is determined by using similarity profiles based on the calculated height and width in the crosswind directions. Mixing of the cloud with the ambient atmosphere is treated by using the entrainment concept. Within SLAB's mathematical framework of heavy-gas dispersion, there is a natural progression toward neutrally buoyant trace-gas dispersion allowing for calculations down to the lowest-desired concentration levels. The main advantage of SLAB over more complex heavy-gas models is its low computing cost. Typical simulations require only a few seconds on a CDC 7600 computer or a few minutes on an IBM microcomputer.

Contact: Donald L. Ermak

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 bilinear 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.

Contact: Stevens T. Chan, Philip M. Gresho

FETISH Model

This two-dimensional 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—either of which allows complex domains to be modeled. 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.

Contact: Philip M. Gresho, Robert L. Lee

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.

Contact: Stevens T. Chan, Philip M. Gresho

HTCM (Hydrodynamic Thermal-Capillary Melt) Model

In support of the Laser Program at LLNL and in conjunction with the Chemical Engineering Department at Massachusetts Institute of Technology, a code has been developed to aid in the understanding of the physical processes occurring in the hydrodyamic melt associated with the growth of large, single-oxide crystals from the melt. The model uses the finite-element method to solve for the following variables simultaneously in an axisymmetric geometry: the velocity, pressure, and temperature in the melt; the temperature in the metal crucible that contains the melt; the shape of the free-surface (melt-to-ambient interface); the shape of the melt-solid (crystal) interface; and the radius of the growing crystal. The model will also be used to help design new apparatus needed for the production of crystals that are larger than any that have been grown by conventional methods.

Contact: Philip M. Gresho, Jeffrey J. Derby

Global Climate Models

LLNL/Community Climate Model

Two versions of the National Center for Atmospheric Research (NCAR) general circulation model, CCM0B and CCM1, have been transferred to the LLNL computer system. Compared to the NCAR-supplied version, the speed of CCM0B has been increased twofold by development of improved memory-management routines; a similar effort for CCM1 is underway. In CCM0B, parameterizations were added to allow aerosols to be included in the radiative transfer routines, and the model is now coupled to GRANTOUR for interactive radiative/microphysical/dynamical simulations. A number of enhanced versions of CCM1, including interactive ocean-surface temperature computations and improved boundary-layer and surface-hydrology modeling, are being developed.

Contact: Curtis C. Covey

LLNL/Oregon State University General Circulation Model

The modified LLNL/OSU GCM is being used as a tool for understanding climate model validation with satellite data and for developing a methodology for model intercomparison. The model has been used to explore causes of the differences among climate models, focusing specifically on differences in cloud forcing and cloud properties. A version of the model coupled to a two-level mixed-layer ocean model produced a southern oscillation.

Contact: Gerald L. Potter

Oregon State University/GRANTOUR General Circulation Model

The GRANTOUR species-transport model and the OSU/LLNL GCM 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. Another version of GRANTOUR treats the global wet and dry deposition of nitric acid resulting from global sources of NO_x and a simple chemistry. This model is run in its uncoupled mode with OSU/LLNL GCM meteorology.

Contact: Steven J. Ghan, John J. Walton

Two-Dimensional Climate Model

A new, essentially two-dimensional atmospheric model is being developed for the purpose of studying the zonal character of climate and, more generally, atmospheric flow in a vertical plane. This hydrostatic model has already been used to study unstable radiative-dynamical interactions (that may, for example, provide a means of lofting a smoke cloud to greater heights). The model is currently being modified to include the processes thought to be most important in determining global climate. In this respect the model will be similar to the Livermore Statistical-Dynamical Climate Model. The new model, however, will include improved radiation codes and a new method to approximately account for the diurnal cycle and land-ocean differences; this should reduce the computational effort required for simulating climate changes that occur over decades. The model will eventually provide a capability of studying climate-chemistry interactions when it is linked with the two-dimensional atmospheric chemistry model.

Contact: Karl E. Taylor

Statistical-Dynamical Climate Model

The Livermore Statistical-Dynamical Climate Model (LSDM), also referred to as ZAM2, is a two-dimensional, Eulerian, thermodynamic model of Earth's atmosphere-surface-ocean system in the meridional plane. 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 been used to test the response to increased atmospheric CO_2, arctic soot, volcanic aerosol injections, and other perturbations.

Contact: Michael C. MacCracken, Karl E. Taylor

Appendix E. LGF Program Overview

History

In 1977, the DOE established the Liquefied Gaseous Fuels (LGF) Program to develop methods to predict the consequences of an accidental release of hazardous materials, to perform large-scale experiments to validate these predictive methods, and to evaluate methods for reducing the consequences of possible releases. The original DOE program focused on the hazards associated with large-scale releases of liquefied natural gas (LNG), but was broadened in 1979 to include other fuels, such as liquid propane gas and ammonia, and has since been expanded further to include toxic liquefied gases in general. Since the accident at Bhopal, India, concern over the consequences of a large-scale accidental release of toxic materials has increased. One result of this growing concern has been an increased interest in conducting tests with these materials at the new DOE Spill Test Facility and in using LLNL computer models of dense-gas dispersion for predictive purposes.

Field Testing

LLNL first became involved with large-scale field testing of LNG in 1978 at China Lake, California, and was responsible for conducting extensive LNG tests in 1980 and 1981. During that time, LLNL put together a multidisciplinary team of scientists and engineers, including an integrated analytical and experimental effort, to work on the complex and interdisciplinary phenomena involved when a hazardous substance is released into the environment. The LLNL team built an extensive and flexible data-acquisition system and sensor array for conducting both field tests and several mathematical dispersion model studies. These models were used for comparison with test results and ultimately for prediction of the consequences of an accidental release into the atmosphere. In 1982, when the test facility at China Lake was shut down, the U.S. Coast Guard and The Fertilizer Institute asked LLNL to complete the ammonia testing program, which they had begun several years before. Also that year, the U. S. Air Force asked for testing to determine the consequences of releases of N_2O_4, a missile fuel oxidizer. LLNL conducted the ammonia and N_2O_4 spill tests in the summer of 1983 using tanker trucks and a temporary facility at the DOE's Nevada Test Site (NTS).

The results of this testing have been both surprising and informative. They have revealed unique dispersion behavior associated with the density, chemical reactivity, and thermodynamics of the release. Essentially all of the ammonia released flashed into aerosol and vapor and was transported downwind. Measured gas concentrations at distances up to 3 km (2 mi) downwind exceeded standard Gaussian-dispersion-model predictions by up to a factor of ten. The presence of large quantities of aerosols created by flashing two-phase flow during the release contributed to this discrepancy. More sophisticated models appear to do better with these predictions when the effects of aerosols are included. Thorough validation through careful comparison to experimental data are still needed. Several industrial organizations have been very interested in these test results, but no systematic analysis of the data has yet been performed.

The DOE research program was terminated in 1982. However, shortly thereafter, Congress directed the DOE to construct a spill test facility. Many industrial organizations had benefited from the program's past work and had indicated that they would continue to support the research if the DOE would construct a facility. In 1983 Congress provided the initial funding to construct a suitable facility.

Early in 1984, after an extensive site-selection study, NTS was chosen as the site for the permanent test facility, and construction was begun. The facility is capable of withstanding tests involving up to 200 m^3 (54,000 gal) of cryogenic materials, such as LNG, with release rates as high as 100 m^3/min, and up to 90 m^3 (24,000 gal) of ambient temperature materials, such as ammonia and chlorine, at pressures up to 300 psi and at release rates up to 20 m^3/min. Extensive diagnostic instrument arrays allow acquisition of data from source rate, atmospheric dispersion, mitigation, and combustion/explosion studies regarding the large number of hazardous materials of concern to industry, government, and the general public. These data can be used to validate models, which can then be used with confidence to predict the consequences of accidental releases. Data concerning the effectiveness of emergency response and hazard mitigation techniques and equipment can be obtained to assure industry, public authorities, and government agencies that these techniques will work in the event of an accident. Validated predictive models will also tell industry and the authorities what the consequences of an accidental release will be and how big an area would be affected in the event of an accident.

A successful series of six hydrogen-fluoride (HF) spill tests was performed for Amoco at the new facility in the summer of 1986. The preliminary results have been very impressive; they indicate that under certain conditions of temperature and pressure, HF releases flash into vapor and aerosol droplets in such a way that the entire mass of material is transported downwind. Preliminary results indicate good agreement with our dispersion models when the source strength is known and thermodynamic effects are included. These results are very similar to those obtained with ammonia. The 1986 tests also involved the evaluation of several water-spray curtain configurations, which may be helpful in combating an accidental release, should one occur. Reduction, validation, analysis, and publication of the data from these tests is still underway, with the test sponsors participating jointly with LLNL in the process.

During the summer of 1987, an ambitious program was conducted at the new facility at NTS under the sponsorship of the Gas Research Institute and the Department of Transportation. The purpose of the program was to evaluate the effectiveness of a large (10-m × 44-m × 88-m) vapor curtain for mitigating the consequences of a large LNG spill. This was an extensively instrumented test series with the primary purpose of gathering data that could be used to validate wind-tunnel and mathematical models.

A number of other organizations are at various stages in planning activities at the facility. An HF industry group will be sponsoring water-spray mitigation experiments in 1988 at NTS. An industrial group of chlorsilane manufacturers and users is working with us on a program for 1989. The Chlorine Institute has completed a testing protocol, and the Chemical Manufacturers Association Phosgene Panal is also considering a program. Oak Ridge and DOE contractors who handle UF_6 are also possible future participants. A chemical reaction between UF_6 and atmospheric water vapor results in the formation of HF. This process was the culprit in the recent accident at Gore, Oklahoma. We have been in touch with the DOE, the NRC, and the contractors operating their facilities, regarding the UF_6 issues. We will continue to work with them on this. Several organizations have expressed interest in continued ammonia testing but have not yet focused on a clear course of action. Good results from past research and a clear need for more information have prompted work at the facility. Testing will, in turn, promote further improvements in the theory and computer models, additional lab-scale tests, and wind tunnel work, all of which will eventually lead back to more field testing until these problems are solved.

Dispersion Models

The LLNL Liquid Gaseous Fuels Program has developed two state-of-the-art atmospheric dispersion models called FEM3 and SLAB. Both of these computer models incorporate mathematical

descriptions of the physics of heavy-gas dispersion. These physics include: gravity spread, the effect of density stratification on turbulent mixing, and ground heating into the cloud, as well as the resultant effects on density stratification and turbulence.

Of the two codes, FEM3 provides the more detailed and complete description of the physics involved in dense-gas flows. It simulates the dispersion of a release gas by solving the time-dependent, three-dimensional conservation equations of mass, momentum, energy, and species, along with the ideal gas law for the equation of state. In addition, it can treat flow over variable terrain and around obstructions, such as cylinders and cubes. Turbulence is treated by using a K-theory submodel, and heat transfer between the ground surface and the vapor cloud is also accounted for. Since it is fully three-dimensional, FEM3 can simulate cloud dispersion involving complicated flow and cloud structures, including the vortices typical of dense-gas flows; cloud bifurcation that has been observed with heavy-gas releases under low wind speed; stable ambient conditions; and cloud deflection caused by sloping terrain. FEM3 can also model both instantaneous sources and continuous releases. Furthermore, a simple phase-change submodel based on local thermodynamic equilibrium is available for handling the phase transition between vapor and liquid. An early version of the code (with a subset of the above capabilities), together with a user's manual, was released to the Argonne code center in 1983. A version with all aforementioned capabilities and updated documentation is being produced under U.S. Army sponsorship.

The SLAB model solves the crosswind-averaged equations for the conservation of mass, species, downwind and horizontal crosswind momenta, and energy. SLAB also solves an additional equation for cloud width and the ideal gas law equation of state. In addition, the current version of this model includes the steady-state assumption for continuous releases. Thus, the code is one-dimensional with downwind distance being the independent variable. However, since cloud width and height are also calculated, the mode is, in this sense, quasi-three-dimensional. The crosswind concentration distribution is determined by using similarity profiles based on the calculated crosswind height and width. Mixing of the cloud with the ambient atmosphere is treated by using the entrainment concept. The main advantage of the SLAB code is its low computing costs. Typical simulations require only a few seconds on a CDC 7600 computer, or a few minutes on an IBM micro-computer. SLAB is widely used but not well documented. Improved documentation, including a user's manual, is currently being generated under sponsorship by the American Petroleum Institute and the U.S. Air Force. Also included in this work is the development of an instantaneous-source and puff-dispersion version of SLAB to complement the existing continuous-source, steady-state capabilities.

Model Development

Source Improvements

Our numerical models were developed with two main release sources in mind—evaporating ponds and instantaneous vapor releases. Other types of sources are also of considerable practical interest; two that we have not considered are jet and stack releases. Many toxic chemicals are stored under pressure. When an accidental release occurs under these conditions, the source is usually a jet release, often a two-phase, droplet-plus-vapor jet release. Stack releases are common in the chemical process industry, both for routine and accidental releases. The main difference with this type of release is that it occurs at an elevated height. Dense gases released from this type of source will experience cloud rise due to the initial inertia of the existing gases, followed by cloud falling. After contact with the ground, the gravity effects of cloud falling, which involve only vertical motion, shift to gravity flow, which involves both vertical and horizontal flow. Methods for treating both types of sources—jet and stack releases—are under consideration.

Turbulence Submodel Improvements

The current FEM3 turbulence submodel is an equilibrium K-theory model in which the diffusion coefficient is based on the local cloud characteristics. This version is a fourth-generation model and is about as sophisticated as can be achieved without going to a higher-order turbulence model. Equilibrium models have inherent limitations regarding the physical phenomena they are capable of treating. Two practical and important cases that are beyond these limits are the effects resulting from the flow over objects and flows involving jet releases. To treat these effects, a higher-order turbulence model is needed that includes turbulence transport, creation, and destruction. Future efforts on our turbulence submodel will be directed towards developing this capacity.

Emergency Response Capability

Methods for dealing with cloud dispersion and more complex flows, for example, methods that simultaneously treat variable terrain, variable wind and meteorological conditions, dense gas effects, and normal ambient meteorological effects, all within a single code, are also under consideration. This degree of complexity naturally requires compromises in the level of physical sophistication used in each individual submodel. We are seeking methods that realistically treat all of these interacting effects in a real-time manner using available computer technology.

Model Validation and Application

Model validation is a continuous and ongoing process as new sources, types of gases, and more complicated situations for simulation are considered. Over the past few years, the predictions from both the FEM3 and SLAB models have been compared with the data obtained from a variety of field-scale experiments. These include the Burro and Coyote series of LNG dispersion experiments and the Eagle series of nitrogen-tetroxide spill tests conducted by LLNL. They also include the refrigerated-liquid-propane spills conducted by Shell Research Limited at Maplin Sands, England, the LLNL ammonia and hydrogen fluoride spill and dispersion experiments, and the British Health and Safety Executive Thorney Island Trials. From all of these tests, 26 were chosen as "bench mark" data sets with the results summarized and published in a report. In addition to the bench mark data sets, a methodology for evaluating heavy-gas dispersion models was developed under U. S. Air Force sponsorship.

Appendix F. Publications

Journal Articles, Reports, and Book Chapters

Atherton, C. S., and J. E. Penner (1987), "Nitrogen Oxide Transformation in a Tropospheric Model," *Tellus*, in press; also Lawrence Livermore National Laboratory, Livermore, CA, UCRL-96343.

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Barnett, T. P. (Scripps Inst. of Oceanography), and M. E. Schlesinger (Oregon State University) (1987), *Detecting Changes in Global Climate Induced by Greenhouse Gases*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-15919.

Broyles, A. A. (1987), *The Dependence of the Mortality for Man on Gamma Radiation Dose*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-96818.

Cederwall, R. T., and K. R. Peterson (1987), *Meteorological Modeling of Arrival and Deposition of Fallout at Intermediate Distances Downwind of the Nevada Test Site*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-96150.

Cess, R. D., and G. L. Potter (1987), *A Methodology for Understanding and Intercomparing Atmospheric Climate Feedback Processes within General Circulation Models*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-97635.

Covey, C. C., and E. Barron (1987), *The Role of Ocean Heat Transport in Climatic Change*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-96940.

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Appendix G. Seminar Speakers

William Chameides, Professor of Geophysical Sciences, Georgia Institute of Technology, "Rainout and Washout in the Atmosphere and in a General Circulation Model," October 9, 1986.

George Baker, Defense Nuclear Agency, "The Implications of Atmospheric Test Fallout Data for Modeling Nuclear Winter," November 18, 1986.

Tony Slingo, British Meteorological Office and the National Center for Atmospheric Research, "The Effect of Cloud Radiative Forcing on the NCAR Community Climate Model," December 1, 1986.

Robert Ellingson, Professor of Meteorology, University of Maryland, "Sensitivity of the NMC Weather Forecast Model to Atmospheric Radiation," December 17, 1986.

Ron Koopman, J-Group, LLNL, "Atmospheric Dispersion of Large-Scale Spills," December 18, 1986.

Michael Ghil, Professor of Atmospheric Sciences and Geophysics, UCLA, "Ice Ages: When and Why," February 2, 1987.

John Leone, G-Division, LLNL, "Finite Element Planetary Boundary Layer Modeling: A Status Report," February 26, 1987.

Peter Gleick, MacArthur Foundation Fellow in International Security and Visiting Research Scholar, Energy and Resources Group, U. of Calif., Berkeley, "Climatic Change and the Effects on California's Water Resources: What Do We Know and What Should We Do?" April 2, 1987.

Sultan Hameed, Professor in Department of Mechanical Engineering and Laboratory for Planetary Atmospheres Research, SUNY Stony Brook, "Simulation of Global Wet and Dry Deposition of Nitric Acid in a General Circulation Model," April 16, 1987.

Bryan Weare, Professor in Land, Air, and Water Resources, U. C. Davis, "Comparison of Radiation Calculations in the UCLA GCM with Observations," May 1, 1987.

Jim Kasting, Research Scientist, Space Science Division, NASA Ames Research Center, "Climate Evolution on Venus, Earth, and Mars," May 7, 1987.

Su-Tzai Soong, Professor in Land, Air, and Water Resources, U. C. Davis, "A Numerical Simulation of the Effect of Steep Topography on Air Flow and Precipitation," May 19, 1987.

Robert Cess, Leading Professor of Atmospheric Sciences in the Laboratory for Planetary Atmospheres Research, SUNY Stony Brook, "A Simple Strategy for Intercomparison of Atmosphere-Climate Feedback Processes within General Circulation Models," May 27, 1987.

Bal Raj Sehgal, Senior Scientific Advisor, Nuclear Power Division of the Electric Power Research Institute (EPRI), Palo Alto, "EPRI Source Term Program," June 12, 1987.

Bill Porch, G-Division, LLNL, "Long Path Spectroscopic Measurements of Pollutants across San Francisco Bay," July 8, 1987.

Thomas Vonder Haar, Director of the Cooperative Institute for Research in the Atmosphere at Colorado State University, "The International Satellite Cloud Climatology Program (ISCCP)," July 16, 1987.

Milo Dorr and Alice Koniges, Computations Department, LLNL, "Two Recent Advances from Computations Relevant to Numerical Modeling," July 21, 1987.

Jae Edmonds, Battelle Pacific Northwest Laboratory, "Uncertainty in Future CO_2 Emissions," August 10, 1987.

Edward J. Kansa, Earth Sciences Department, LLNL, "Improvements to Spatial Approximations in Computational Fluid Dynamics Using Multiquadrics," August 27, 1987.

Richard Eckman, Cambridge University, "Uncertainties in Two-Dimensional Atmospheric Modeling," August 31, 1987.

Appendix H. Acronyms and Abbreviations

Acronym	Meaning
1-D	One-Dimensional
2-D	Two-Dimensional
3-D	Three-Dimensional
ADPIC	Atmospheric-Diffusion Particle-in-Cell
AFGWC	Air Force Global Weather Central
APCA	Air Pollution Control Association
ARAC	Atmospheric Release Advisory Capability
ASCOT	Atmospheric Studies in Complex Terrain
BAAQMD	Bay Area Air Quality Management District
BES	Department of Energy/Office of Basic Energy Sciences
CAP	Containment Atmosphere Physics
CAPTEX	Cross-Appalachian Tracer Experiment
CCM1	National Center for Atmospheric Research/General Circulation Model
CMA	Chemical Manufacturers Association
CPS	Continuous-Point-Source
CSU	Colorado State University
CZ	Czochralski
DNA	Defense Nuclear Agency
DOD	Department of Defense
DOE	Department of Energy
DOT	Department of Transportation
DP	Defense Programs
EH	Department of Energy/Office of Environmental Safety and Health
EPA	Environmental Protection Agency
ER	Department of Energy/Office of Energy Research
FAA	Federal Aviation Administration
FE	Department of Energy/Office of Fossil Energy
FEM	Finite-Element Modeling
FEM3	3-D Finite Element Model
FY	Fiscal Year
GBL	Ground-Based Laser
GCM	General Circulation Model
G-Division	Atmospheric & Geophysical Sciences Division
GPP	General Plant Projects
GRANTOUR	Lagrangian Parcel Advection Code
IBM	International Business Machines
ICRCCM	Intercomparison of Radiative Codes in Climate Models
ICSU	International Council of Scientific Unions
IR&D	Institutional Research and Development
J-Group	Liquefied Gaseous Fuels Program
LIRAQ	Livermore Regional Photochemical Air Quality Model
LGF	Liquefied Gaseous Fuels
LLNL	Lawrence Livermore National Laboratory
LNG	Liquefied Natural Gas
M/A	MATHEW/ADPIC
MATHEW	Regional Diagnostic Flow Model
NAPAP	National Acid Precipitation Assessment Program
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research

NR	Naval Reactors
NRC	Nuclear Regulatory Commission
NTS	Nevada Test Site
OHER	Department of Energy/Office of Health and Environmental Research
OMA	Department of Energy/Office of Military Applications
OSU	Oregon State University
PIC	Particle-in-Cell
SLAB	1-D Dense-Gas Dispersion Model
SUNY	State University of New York
TMI	Three Mile Island
UARS	Upper Atmosphere Research Satellite
UNEP	United Nations Environment Programme
WMO	World Meteorological Organization
WSR	Physics Department/Weapons Special Research