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**PROGRAM REPORT - FY 1973
ATMOSPHERIC SCIENCES GROUP
PHYSICS DEPARTMENT
LAWRENCE LIVERMORE LABORATORY**

August 28, 1973

Prepared for U.S. Atomic Energy Commission under contract No. W-7405-Eng-48

**LAWRENCE
LIVERMORE
LABORATORY**

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PROGRAM REPORT - FY 1973 ATMOSPHERIC SCIENCES GROUP PHYSICS DEPARTMENT LAWRENCE LIVERMORE LABORATORY

Abstract

The research program in the atmospheric sciences at the Lawrence Livermore Laboratory has been consolidated under the purview of a newly formed Atmospheric Sciences Group in the Physics Department. The program is responsive to a number of national needs; they are outlined for both civil and military categories. Our capabilities

at the Laboratory that are unique for this endeavor are enumerated. The scope of current and developing projects is described together with an indication of significant findings of the work. The prospects for FY 1974 are discussed in terms of growing potential to fulfill assignments from the AEC and other governmental agencies.

Introduction

During the course of the last year, a new activity developed at LLL that has given added impetus to studies in the atmospheric sciences, particularly in the development of numerical modeling techniques. A separate Atmospheric Sciences Group (G-Group) was established in the Physics Department to provide new focus for the Laboratory's participation in the national efforts in this field. Formed from a nucleus of researchers in the Fluid Mechanics Group of the Earth Sciences Division and the Hydrodynamics Group of the Theoretical Physics Division, the new organization has the responsibility for an integrated Laboratory program for

both the AEC and other agencies.

The Group Leader is Dr. J. B. Knox. The Atmospheric Sciences Group is a part of the Physics Department, which is headed by Dr. R. N. Keeler and is under the general guidance of Dr. E. Teller, Associate Director for Physics at LLL. For work in the category of environmental studies, the Group acts as an operating arm of a program directed by Mr. R. C. Maninger under the general guidance of Dr. M. M. May, Associate Director-at-Large. The Group now consists of approximately twenty professionals, eleven contributing scientists, and administrative support.

Relationship of Our Work to National Needs

The current research program at the Laboratory in the atmospheric sciences is intended to address certain identified national needs. The following discussion of needs is not intended to be all-embracing, but rather to outline the patterns on which research objectives are now established or will be formulated.

CIVIL

For conventional (non-nuclear) air pollution problems, there is a recognized need in the air pollution community for methods, techniques, and numerical simulation models to accomplish the following:

1. The evaluation of land use plans that in the long term lead to environments that satisfy the ambient air quality standards now adopted or those that may be developed in the future.
2. The determination and evaluation of the effectiveness of various control strategies developed to deal with episodes, kind and deployment of emission controls, and other suggestions bearing on the reduction of emissions and their effect on air quality.
3. The estimation of levels of pollution in which backgrounds are expressed as frequency distributions of surface air pollutants.
4. The prediction of air quality on a regional basis such that adequate forewarning can be given for implementing control strategies

against episode conditions. This implies that regional scale meteorological prediction capabilities be ultimately developed; the intent would be to apply such a capability to the operational forecasting of air quality of selected regions judged to be approaching or entering high air pollution potential.

For regional nuclear pollution problems, the need for the development of regional modeling of multi-sources of emissions, their transport, diffusion, deposition, and the drives of various modes of exposure to man has long been recognized as requiring improved or advanced techniques. The late AEC Commissioner Theos Thompson was among the first to recognize (1970) the potential for adapting computational models to the real time estimation of dose exposure of U.S. population groups from operating emissions of the nuclear power industry or AEC facilities. It is now widely held that there is a need to provide: (a) advisory information on dose commitments and possible counter-measures against massive accidental releases of radioactive or toxic materials, (b) the documentation or estimation of the dose commitments associated with the normal operating releases from nuclear facilities or AEC sites, and (c) assistance to the Regulatory Directorate in special assessments of sites or in improvement in the application of guidelines to complex sites. An example of this latter type of support might well include site evaluation in regard to diffusion environments associated with heterogeneous surface

boundary conditions with off-shore sitings or mesoscale meteorological modeling supporting this same need.

It is generally well recognized that new technologies and energy policies need to be evaluated as to their environmental consequences prior to the commitment of large sums of money to their development or implementation. The effects of such policies are usually regional or global in their scale and may have long term impact on terrestrial climate. The present LLL participation in the Climatic Impact Assessment Program (CIAP) of the Department of Transportation is an illustration of the type of analytical-method-model development needed to assess problems associated with an SST fleet, strategic nuclear exchanges, or the accumulation of anthropogenic pollution from power generation, agriculture, or other alterations of the earth's surface. Tools developed for CIAP can be and should be extended to investigate:

- Global balances and budgets of important atmospheric trace constituents (H_2O , C, N, O, O_3), aerosols, and particles.
- Radioactive pollutants from the nuclear fuel cycle and/or nuclear testing.

Investigations of mechanisms of terrestrial climatic change have been a subject of intellectual curiosity for a number of years. There is now an awareness, which in some circles is construed to be a pressing need, to instigate major climate studies whose success depends on availability of advanced computers. Man is becoming aware of the fact that he will soon, if not already, have within his grasp the power to

affect global scale changes. There is a consensus in the scientific community that climate studies should be actively pursued in the next decade for these reasons and others. Such studies should include, but not be limited to, the following:

- Simulations of past climatic states using appropriate boundary conditions.
- Simulations of present climate distributions and possible mechanisms of climatic change.
- Studies of the geophysical and atmospheric description of the life history of an interglacial period, the distribution of climate and its variability during interglacials, and the comparison of the former to our present interglacial condition.
- Exploration of the anthropogenic contribution to climate change through combined effects of CO_2 , particulate loading, waste heat, or alterations of the earth's surface by urbanization, deforestation, and agricultural practices.

The need for the assessment of the pollution of aquatic systems with conventional pollutants, radioactive pollutants, waste heat, or dredge spoils has led to a need to transfer the more advanced modeling concepts (e.g., couple hydrodynamics and kinetics) from atmospheric research to aquatic systems. Three-dimensional simulation methods are at this date completely lacking in the aquatic system simulation area of research.¹

Global scale studies of the limits of growth and the future state of man have been pursued by an MIT group. Their results have been strongly criticized by

economists and physical scientists for many reasons. Essentially the shortcoming is that a complex problem has been treated in an oversimplified manner, the results of which are inconsistent, depending on compartmentalization of the factors and the kind or number of feedback loops or processes included in the model. Investigations by Kadanoff² and Boyd³ show that, as a result of differing compartmentalizations of the problem, which in turn lead to different numbers of feedbacks, the solution of such system models can lead to diametrically opposite conclusions. Solutions were also shown to be very sensitive to boundary conditions and to the functional forms assumed for critical relationships in the model. It has been suggested that the MIT studies might have considered the effect of pollution abatement for a small fraction of the GNP on the exponential growth of pollution. That the MIT group has done an apparently incomplete investigation of the long term predicament of man does not necessarily mean that work in this area is not needed.

There is, however, an alternative way to begin, namely, to develop the desirable conditions we seek for our global environment; i.e., to use our analytical-physical tools emerging from the CIAP and other programs to investigate the corresponding and consistent emission levels, the parallel controls required, the optimum means of providing energy, and limits, if required, on per capita energy consumption. The conditions under which the population could grow while maintaining environmental quality could, in principle, be explored in such a study.

MILITARY

In addition to the broadly based civil needs, there are identified national security needs to be addressed. This discussion is based primarily on research topics currently under study.

For tactical nuclear warfare modes there is the need for the development of improved methods of assessing the potential dose commitments for wet depositions of cloud inventories of radioactive debris as a function of seasonal diffusion and scavenging environments, mode of employment, and yield and content of the available weapon inventory. For the same purpose, there is a need for the investigation of dry deposition models of exposure for comparison and for estimating the hazard at long ranges.

For strategic exchange environmental problems, the impact of the oxides of nitrogen injected into the stratosphere during a nuclear exchange needs to be evaluated in a realistic manner. Such studies must focus on the alteration of the UV radiation reaching the earth's surface and the attendant biological implications and effect on man, as well as the potential for altered stratospheric thermal structure, which may lead eventually to climatic changes of a magnitude unknown at this time.

For prediction of nuclear weapon delayed effects, basic efforts in numerical hydrodynamics need to be initiated in regard to three-dimensional solutions for more accurate assessments of nuclear cloud height, debris distribution at stabilization, and cloud interaction.

For military environmental problems, better definitions of liquid and solid hydrometeor distributions are needed in

a form useful to military decision makers. More comprehensive and focused research on resuspension of toxic and non-toxic

materials (including plutonium at some AEC sites) is needed in order to achieve a solution on a useful time scale.

LLL Modeling Capabilities

The primary means in the Atmospheric Sciences Group of meeting the research objectives established in response to national needs are numerical analysis and modeling techniques. Unique modeling capabilities of the group are listed below.

1. ZAM2 is a two-dimensional, Eulerian thermo-dynamic model of the earth's surface-atmosphere system in the meridional plane. The model considers a moist atmosphere and includes such effects as solar and longwave radiation, variable cloudiness, precipitation, trace species balances, surface interactions, variable sea ice extent, and mountains. The model is relatively fast running, requiring several hours of 7600 time to simulate one year of terrestrial climate.^{4,5}
2. 2BPUFF is a two-dimensional, axially symmetric, Lagrangian code for calculating the anisotropic diffusion of fine particles of gases in a frame of reference moving with the center of the cloud of particles or gas. The diffusion coefficients can be time dependent. An Eulerian grid is used on the earth's surface to keep track of the cloud position and to provide the framework for bookkeeping on air concentrations during the passage of the moving cloud.^{6,7}
3. The LLL air pollution model is a two-dimensional, time-dependent multibox model used to calculate the mean concentration and surface concentration of passive and photochemical pollutants. The present method of solution is based on a modified version of Gear's technique for solving large sets of stiff ordinary differential equations.^{8,9}
4. A three-dimensional particle diffusion code is being developed to calculate the transport and diffusion of a puff or plume in a transient atmospheric boundary layer. The model is based on the Particle-in-Cell (PIC) concept, with the hydrodynamical aspects of the conventional PIC deleted. This code is intended to supplement the 2BPUFF code in that the new model will predict cloud shape, as well as concentrations, at early and late times in stratified shear flow.
5. An improved three-dimensional mass-consistent wind field submodel is currently being developed and tested. The purpose of this model is to calculate a three-dimensional non-divergent wind field solution for a regional air shed such that the solution satisfies the kinematic boundary conditions of complex terrain, the time and space dependent behavior of the inversion capping the mixed layer, the

conservation of mass, and the wind observations during a specified period. The output of this sub-model will be used to calculate the advective and diffusive fluxes in a regional air pollution simulation model.¹⁰

For studies in the stratospheric regime for the CIAP, models 6, 7, and 8 have been developed.¹¹

6. A dispersion and transport model consisting of a group of single-plume and flight corridor models to describe the wake concentration history in the transition region from the stabilized aircraft wake to the global scale. These models are designed to determine the effects on the quasi-equilibrium concentrations characterizing a flight corridor caused by (a) early period concentrated wake kinetics, (b) the spatial and temporal distribution of wake injections (i.e., the injection schedule), and (c) dispersion of individual wake plumes by scale-dependent eddy diffusion and/or shear.

7. The coupled kinetics and transport modeling includes one- and two-dimensional numerical models to simulate, using prescribed mean winds and eddy diffusion coefficients, vertical and latitudinal dispersion of stratospheric tracers. These models incorporate the kinetics models (described below) with interactive radiation transport, but allow no feedback of the tracers on the transport. These models are intended to compute quasi-equilibrium distributions of trace species

resulting from prescribed stratospheric injection schedules and ambient transport kinetics.

8. A stratospheric kinetics model simulates the chemical and photochemical kinetics of the stratosphere. The model includes the kinetics of a well mixed cell, gaseous absorption and concomitant attenuation of the downwelling solar spectrum, and application of advanced mathematical methods. Considerable attention is directed toward the development of a capability to evaluate the following:

- a. sensitivity of reaction mechanisms to deficiencies in our knowledge of the solar constant, reaction rates, quantum yields, reaction ensemble, and reactant concentrations.
- b. the effect of using diurnally and seasonally varying solar flux (as opposed to time-averaged solar flux), and
- c. the feasibility of developing reduced reaction sets for incorporation in more complex models, permitting interaction with other atmospheric processes.

Working in conjunction with other Laboratory divisions, including Chemistry and Biomedical Research, we have developed two additional tools. The first is a set of dose conversion constants. The complete set of constants for all significant nuclides and all modes of exposure has been reviewed and updated. The information is kept on tape files and is available for calculating potential dose to man. The second jointly developed tool is the CPS code. This code calculates the surface air concentration and ground level

deposition from the bivariate Gaussian plume solution for a continuous point source. The output is a two-dimensional display of the surface air relative concentrations (or depositions) for various levels of probability of occurrence. When coupled with source term information and appropriate dose conversion constants, the dose commitments from the significant nuclides by various

modes of exposures can be estimated on an organ by organ basis.

All of the above mentioned tools permit the performance of a variety of environmental assessments and constitute a strategic base for launching new projects directed at filling significant technical needs. Our recent experience in the use of these analytical tools is outlined in the following section.

Progress on Current Projects for FY 1973

Major atmospheric science research projects during FY 1973 at LLL included: (a) the study of the transport and diffusion of radionuclides from source to receptor areas (including their mechanisms of decay, means or removal from the atmosphere, and modes of deposition); and (b) numerical simulation of regional air pollution from multiple sources of either conventional or radioactive pollutants. Work on the development, verification, and application of a hierarchy of models for solving specific applied research problems was performed. Special projects on meteorological aspects of nuclear weapons effects were carried out, and environment impact statements for LLL were prepared.

REGIONAL MODELING

During FY 1973 the Division of Biomedical and Environmental Research (DBER) funded G-Group for two research projects. The first is numerical modeling of regional pollution from nuclear sources, and the second is development of a concept for an Atmospheric Release Advisory

Capability (ARAC). The objectives of the first project are to develop numerical models of regional air pollution that can arise from multiple nuclear sources at a point or in a volume, whether instantaneous or continuous in character. The models include the effects of wind speed and directional shear in the horizontal field, space and time variable transport mechanisms due to advection and eddy diffusion, and space variable surface roughness and terrain. One of the models under development is a specialized model that would, by using computer time economically, be useful in solving regional and continental air pollution problems rapidly in real time. We anticipate that the output of such a specialized model would give surface air concentrations in space and time, as well as unit area depositions of appropriate radionuclides, yielding important information for the calculation of individual and population doses from given releases. The Group has developed two very useful models: an improved mass-consistent wind field model for specifying the winds and mixing depths in the regional boundary layer; and the ADPIC code for calculating

the transport and diffusion of puffs, and plumes in transient, stratified shear flow. We anticipate in the future that these models will be validated, applied to case studies for verification, and utilized in significant studies concerning the evaluation of nuclear accident risks on a probabilistic basis. We also anticipate the use of these models in providing the technical basis for the operation of an atmospheric release advisory center.

ATMOSPHERIC RELEASE ADVISORY CAPABILITY

In regard to the second DBER research project, we expect to complete the development of a concept for Atmospheric Release Advisory Capability (ARAC), Phase I, by September, 1973. In the development of this concept we see that there is a discernible need emerging in the United States for a capability to predict the effects, including dose-to-man, from releases that might arise from a growing nuclear industry and from activities of the AEC. The objective of Phase I is to develop a concept for an ARAC Center for the country based on the present state-of-the-art in meteorological simulation modeling and pathway modeling. It will be necessary to identify deficiencies that may exist in the present state-of-the-art. Within the scope of this work, we expect to evaluate various technical alternatives for meeting this objective. These alternatives will involve the use of meteorological data analyses of forecasts from more than one Federal Agency and from the operators of nuclear power sites. Upon the completion of the concept development, we anticipate that a demonstration phase, Phase II, will be executed.

The operation of the ARAC Center will then be demonstrated in real time against the operational or the simulated accidental releases at an AEC site. With advanced computing systems we expect that, with a modest investment of computer time, an ARAC Center could be placed in operation for the nation in approximately two years. Real time predictive information on estimated maximum individual and population doses with a response on a time scale of several minutes could be provided.

NUMERICAL MODELING FOR CIAP

The Department of Transportation, through its CIAP, is seeking to determine the effects on global climate caused by large numbers of aircraft operating in the stratosphere. The results of these studies will be published as a series of monographs in 1974. As a contributor to that program, LLL has undertaken a number of studies emphasizing numerical model development and application. This is our largest current effort (FY 1973 to FY 1975) in modeling atmospheric processes.

Understanding any problem as complex as the response of the atmosphere to prescribed perturbations requires a thorough mix of observational and theoretical studies, blended through the medium of a numerical model. Experience in the numerical modeling of applied research problems has enabled us to formulate a hierarchy of models, each of which both focuses on discrete sub-problems that deserve individual study and also contributes to the analysis and modeling of the larger, overall problem.

Five distinct modeling efforts are underway. Three of these are based on the different scales of atmospheric motion. The other two address stratospheric kinetics and radiation transport. The five different modeling efforts, some of which involve more than one model, are:

1. Dispersion and transport model.
2. Global kinetics and transport model.
3. Zonal Atmospheric Model (ZAM2).
4. Stratospheric kinetics model.
5. Radiation transport model.

In particular, these models treat the diffusion and transport of aircraft exhaust emissions and the photochemical reactions of these pollutants with ozone and other components of the ambient atmosphere, focusing on the mechanisms and results of possible modifications in the composition of the stratosphere. From these calculations, induced changes in the global climate and ultraviolet radiation at the earth's surface will be investigated.

While our first year efforts emphasized model development, during the second year our attention will be directed toward model application to validation, sensitivity, and perturbation studies. The scope of these efforts is broad, ranging from kinetic studies in the individual aircraft plume and its interaction with the flight corridor background to global climate studies. As these studies near completion, interaction with other CIAP projects is expected to increase through the cooperative effort of writing the monographs being prepared to document CIAP.

With late 1974 as the target date for completing the CIAP project, we are confident that our models will be useful and well-used tools in developing the required understanding of the atmosphere.

SAN FRANCISCO BAY AREA MODELING

A regional model of the transport and diffusion of nonreactive air pollutants for the San Francisco Bay Region has also been developed at the Laboratory. The model has been used to study the dispersion of carbon monoxide emissions in the Bay Area. Funding has been received to continue the development of this model to include pollutants that take part in photochemical reactions. This work is being done under the RANN Program of the National Science Foundation as a joint effort with the NASA-Ames Research Center and the Bay Area Air Pollution Control District. The resulting model is intended for use as a tool for assessing pollution control and abatement strategies, as required by law, and for investigating consequences of various alternatives in land and resource use in the San Francisco Bay Area.

PRECIPITATION SCAVENGING

The problem of rapid deposition of radioactivity from nuclear debris clouds at various distances from ground zero has been addressed in our studies.^{12,13} The results show that high exposure rates could occur in the local region of the burst under the following special circumstances: the radioactivity is distributed in the lower troposphere, it is scavenged at an early time by a rain-bearing system and is rapidly deposited over the ground, and it is confined to a relatively small area. More recent studies have been and are being made at LLL to make it possible to assess the validity of the results of this earlier publication¹² by considering in

greater detail the physical processes involved and the extent to which the results may be changed by manmade modifications. The research projects currently underway at LLL that are directed toward quantifiable assessments for the needs of the Defense Nuclear Agency are as follows:

1. A study of the dynamics of cumulus cloud interaction with a nuclear debris cloud to determine possible enhancement or reduction in peak surface concentrations.
2. A study of the microphysical interactions of debris particles with cloud droplets and raindrops to determine rainout and washout efficiencies.
3. A study to determine the feasibility of rendering the debris particles non-wettable, thereby effectively making the rainout coefficient negligibly small.

4. A study of the potential effects of dry deposition due to the detonation of larger numbers of low yield devices within a confined area.
5. The development of a three-dimensional, atmospheric, particle-in-cell code capable of calculating the time-dependent distribution of air pollutants under conditions of turbulent diffusion and wind shear.

OTHER PROJECTS

Other current projects include a study of cloud phenomenology for the Defense Nuclear Agency, environmental investigations for elements of the Department of Defense, and general supporting tasks for the Laboratory, including inputs to environmental impact statements for Laboratory projects.

Prospects for FY 1974

As we enter FY 1974, expansion in the program is already under way. An additional project recently commenced concerns the Transport Phase of the study on reactor safety conducted by the Safety Analysis Task Force under the Chairmanship of Professor Rasmussen of MIT. In response to the stated need of the Task Force, LLL is performing a series of calculations of the transport, diffusion, and dry or wet deposition of a spectrum of accident-vented isotropic inventories (provided by the Task Force) for a variety of sites ranging from the meteorologically simple to the complex. For the selected

sites, the diffusion and deposition environments will be categorized and the probability of each category determined along with its azimuthal distribution, if it is nonsymmetric.

Both the advanced models (the three-dimensional mass consistent wind sub-model and the three-dimensional particle diffusion code) and the CPS code (representing the presently available state-of-the-art) will be used to calculate the relative concentration and relative deposition, dry or wet, if appropriate for the particular isotope. The integrated surface air concentrations and isotopic unit area

depositions will be output as a cathode ray tube graphic presentation for report and intercomparison purposes.

The potential dose-to-man from all significant nuclides and by all modes of exposure (inhalation, submersion, external gamma from deposition, food chains, etc.) are to be calculated; the dose to a given organ from a particular mode of exposure to a particular nuclide is calculated from the time-integrated relative concentration or unit deposition and the appropriate dose conversion constant. The dose commitment to a given organ is estimated by summing over all nuclides and all modes of exposure affecting a given organ. The total organ dose commitments can then be compared to guidelines; associated with each of these commitments is the appropriate probability of the diffusion scenario for the site involved.

New areas are being considered for initiation of research in FY 1974.

In the area of aquatic systems simulation, we have identified two significant problem areas pertaining to sediment transport to which our modeling experience can be applied. These two areas are the numerical simulation of the fate of

dredging spoils disposed of in transient shear flow (requiring the adaptation of ADPIC) and regional sediment transport modeling of the San Francisco Bay.

Discussions have also been held on our potential at LLL for conducting climate simulation research. There is some interest in building a global model of the particulate budget and estimating the effect of the additional particulate loading on wet deposition processes and precipitation processes, for example.

For the AEC a new project has been discussed to do fine-mesh mesoscale modeling. The objective of this research would be to develop a three-dimensional, regional scale (about a 10-km grid interval) numerical model for predicting the meteorological state for 12- to 24-hour periods.

An advanced studies project is now being initiated that involves our computational physics, nuclear effects, and atmospheric science experience.

During FY 1974 the Laboratory may well participate in the formulation of a model capable of reasonable predictions covering the future composition and condition of a mixed conifer ecosystem stressed by oxidant air pollution.

Summary and Conclusions

The Laboratory has been concerned with atmospheric problems since its inception. At first these problems were associated with the nuclear weapons program and included such areas as the radioactive fallout produced by nuclear experiments in the atmosphere and plutonium contamination resulting from

accidents involving nuclear weapons. Later our interests expanded to studying theoretical geophysical hydrodynamics and applied research in the ecological effects of underground Flowshare nuclear explosions and venting. As a result of these responsibilities, the Laboratory has a broad base of personnel and

experience in the many fields necessary for understanding and solving atmospheric problems for different classes of pollutants and sources. In particular, the Laboratory has developed a proven multidisciplinary team to perform numerical modeling of physical, chemical, and transport processes in the environment on urban, regional, continental, and global scales.

A series of projects are now focused under the direction of the newly formed Atmospheric Sciences Group at the Laboratory. The projects cover a wide

spectrum of studies based primarily on numerical analysis of the atmospheric processes. Unique modeling techniques based on Eulerian and Lagrangian grid approaches have been developed; further development of suitable codes is continuing. Continued growth is anticipated both in scope of projects and number of personnel for performance of an expanding number of tasks. While current projects are sponsored in part by AEC, the larger part of the program is now sponsored by other government agencies.

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