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ATMOSPHERIC TRANSPORT AND DISPERSION OF POLLUTANTS
AND RELATED METEOROLOGICAL STUDIES

NOAA/Air Resources Laboratory
DOE/Office of Health and Environmental Research

Final Report for 1990

I. Emergency Response (ER)

A new National Meteorological Support Plan for Federal responses to the release of hazardous materials into the atmosphere is being formulated. The plan summarizes Government agencies' responsibilities for characterizing, validating, identifying, tracking, monitoring, and forecasting the transport and dispersion of released hazardous materials. Under Chapter 2, Agency Requirements and Capabilities, the plan states that Department of Commerce, National Oceanic and Atmospheric Administration (NOAA) research activities in atmospheric transport and dispersion are conducted primarily within NOAA's Air Resources Laboratory (ARL). The DOE is also a participating agency responding to capabilities and requirements.

To fulfill these obligations, ARL is continuing to develop its Immediate Response Program (IRP) composed of:

- (1) Analysis - forecast trajectory models;
- (2) Analysis - forecast transport and dispersion models; and
- (3) Meteorological support - data access and display programs.

Trajectory models are being completely revised for operational use. Trajectories are calculated on an ARL terminal and printer in an interactive mode with NOAA's NAS/9000 mainframe computer at Suitland, MD using analysis and forecast meteorological fields from the National Meteorological Center twice-daily production suite.

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A personal computer (PC) terminal emulator has been developed to link mainframe calculations with user-friendly PC input and tabular and graphical output. The emulator supports operations through a standard modem and tests for specific character strings in the mainframe program that instruct the emulator to take certain actions such as print on and print off for trajectory endpoint tabulation, and save trajectory plots on disc. The emulator also generates map backgrounds consistent with mainframe generated plots, and merges plots and map background for final printed presentation along with printed tabular endpoint locations. A code has also been written and included in certain models that gives a computer written description of a trajectory map. This output has been used for disseminating information on the long-range transport of volcanic ash as a hazard to air operations following a volcanic eruption. Emulator and descriptive codes will be maintained and further developed with changing ER needs.

ARL is currently taking delivery of a satellite-based meteorological data acquisition system from Alden Electronics for purposes of meteorological support to the IRP. The system consists of two parts: a PC-based programmable DIFAX weather chart system (D100), and a menu-driven, window-based software system (MSAT-90) that provides easy access to all of the data from the National Weather Service alphanumeric Family of Services. The D100 receives DIFAX charts from all sources of NWS DIFAX broadcasts. The user has the ability to accept or reject any of the charts available. These charts are stored on the PC and can be called up, displayed or printed with only a few keystrokes. DIFAX charts can also be zoomed or looped to allow detailed analysis of any portion of the chart and any series of charts. The system is capable of receiving, storing and printing charts in a totally unattended mode of operation. The MSAT-90 system also operates unattended; receiving, sorting, and printing programmed products from the NWS alphanumeric Family of Services. The user friendly pull-down windows and quick access data view feature allow the user to obtain any bulletin from the NWS data services within seconds. The data can also be accessed from other programs, such as Fortran programs, to process and display the data for use with unique applications. MSAT-90 runs in a background mode so that other applications can be run on the PC without disturbing the receiving and processing of the data. A full development of this system for ER purposes is proposed for 1991.

II. Transport and Dispersion Modeling

Several analysis and forecast transport and dispersion models are maintained for immediate response usage with continued evaluation ongoing. The Forecast Transport and

Diffusion (FTAD) model is a planetary boundary layer model run on sigma (terrain following) surfaces using forecast meteorology from the NMC Regional Run (Nested Grid Model) downloaded to a PC. The user friendly program outputs forecast surface air concentrations for any location in North America and runs in seconds from the downloaded meteorological data.

Another long-range model, the Hybrid Single-Particle Lagrangian Integrated Trajectory (HY-SPLIT) model, is based on hybrid calculation methods between Eulerian and Lagrangian approaches. A single pollutant particle represents the initial source. Advection and diffusion calculations are made in a Lagrangian framework. However, meteorological input data can either be gridded from rawinsonde observations or archived from the output of an Eulerian primitive equation forecast model. As the dimensions of the initial particle diffuse into regions of different wind direction or speed, the single particle is divided into multiple particles to provide a better representation of the more complex flow field. Air concentrations are calculated on a fixed three-dimensional grid by integrating all particle masses over the sampling time.

A third model, an eight-layer Eulerian transport and dispersion model, is being developed for application on a PC to simulate the global distribution of pollutants. Initial tests were conducted using ^{85}Kr because the number of sources are limited to a few locations and their emissions are documented. The model was able to reproduce the interhemispheric gradient of 3-4 pCi/SCM from uniform initial conditions. Correlation coefficients between model results and measured data were as high as 0.6 but more typically 0.4; still much greater than other Lagrangian source-receptor models. This is primarily attributed to the fact that the model is designed to predict the variations in background concentration as well as plumes although the plumes are considerably damped due to the large grid sizes used in the model. Lagrangian models typically predict excess concentration above background which can result in considerable individual error in day-to-day statistical comparisons. The stability of this Eulerian approach allows emission rates to be estimated for sources that are not well known by determining emissions that are required to match the model results to the measured data. Some practical applications were tested such as determining whether the emission rate assumed for a particular source in the model calculation in conjunction with air concentration measurements can be used to determine the actual emissions. The model results can also be used to estimate global means more precisely by using the model predicted fields as an interpolation function for use with limited spatial measurements. Other uses are estimating time varying ambient background concentrations due to distant sources so that the contribution of low emission local sources can be more easily resolved.

- Model Evaluation

ARL is investigating new techniques for FTAD and HY-SPLIT model evaluation using ANATEX measured concentrations. A new parameter, defined as the factor-of-two distance (D_2), seems to provide the most robust statistics to date on comparisons between calculated and measured concentrations. D_2 is the shortest distance from a sampling site with a measured concentration to a model calculated concentration contour that is within a factor of 2 of the measured value. Since no subjectivity is involved in determining D_2 (as is the case in defining concentration "footprints"), a computer program has been developed to directly calculate D_2 values from gridded model calculated concentrations. D_2 statistics are presented in easy-to-interpret boxplot diagrams for model sensitivity study evaluation and intermodel comparison.

- Vertical Mixing during ANATEX

The ANATEX period provided many cases of tracer release during very stable conditions, typical of many regions in the northern hemisphere during the winter. In many of these releases, model calculations mixed the tracer upward either too rapidly or too slowly, resulting in a subsequent long-range transport trajectory that was not representative of the tracer release. In a study in progress, the aircraft sampling data are being used to compute the actual initial vertical mixing rate, through computation of crosswind integrated concentrations, and comparing them to the mixing that is inferred from model calculations using the NMC Nested Grid Model (NGM) meteorological data. As expected, preliminary results show important differences. Further study will investigate these differences. Not only are vertical mixing rates important, but also the depth of the layer through which the tracer has mixed. For several releases tracer was measured above the boundary layer as defined by the NGM. This may explain some of the difference between the (NGM) calculated and measured concentrations and suggests studying the use of rawinsonde data to calculate the boundary layer height.

- Trajectory Sensitivity to the NGM Data

All the reviewer comments have been satisfied and a paper entitled "Sensitivity of Three-Dimensional Trajectories to the Spatial and Temporal Densities of the Wind Field" will be published in the October issue of JAM. Archived data from NOAA's NGM were degraded both in time and space to determine the sensitivity of calculated trajectories during

the ANATEX period. Trajectories were most sensitive to the temporal resolution, especially for spatial resolutions of 90 and 180 km. At 360 km the coarse spatial resolution dominated the temporal. Relative horizontal transport errors ranged from 5-25% of the travel distance after 4 days travel time. Results showed that transport errors are similar for trajectories computed with a temporal resolution of 2 h on a 90 km grid as on a 180 km grid. This information was directly applied on September 1 when a new archive of meteorological data from the NGM was initiated with a spatial resolution of 180 km and a temporal resolution of 2 h, thereby saving memory and disk space that a 90 km grid would have required. This archive will be used for future transport and diffusion research.

- Absolute Trajectory Error during ANATEX

The above mentioned study of trajectory error has been expanded to include ANATEX ground-level tracer measurements. Tracer concentrations at each measurement site have been subjectively assigned to a release location (St. Cloud or Glasgow) and release day. Center of mass calculations have been made on the 24 h tracer concentrations to infer the "true" trajectory from each tracer release. The true trajectories are being statistically compared with trajectories computed on various meteorological data to determine trajectory sensitivity. Trajectories will be evaluated based on their relation to synoptic conditions existing during transport.

- Trajectory Error from Aircraft Tracer Measurements during ANATEX

Aircraft tracer measurements during ANATEX provided 30 separate trials to evaluate the error of trajectory calculations to the use of dynamic model output meteorological data, 4 per day rawinsondes, and 2 per day rawinsonde observational frequency. Over all events, no significant difference was discernable in trajectory accuracy between the meteorological input data; absolute trajectory error was about 30% of the travel distance. When the trajectories were grouped into similar categories, the least error was observed during regimes of stronger flow, either east or west with errors of 16 to 19%. The largest trajectory errors occurred in weakly defined flows and ranged from 40 to 54%. The NGM data provided the best results when smaller scale flow features, ones that could not be resolved in the rawinsonde network, were present. Rawinsonde data provided the best results when fronts or low pressure systems were present in the vicinity of the tracer release. In 70% of the event the 4/day and 2/day rawinsonde calculation were comparable, suggesting that linear interpolation of the flow field is adequate for most situations. Because the mix of NGM model initialization and forecasts gave comparable results to calculations using rawinsonde data directly, further

experiments can be performed without the costly enhancement of 4 times per day rawinsonde observations.

III. Meteorological Data Archiving

ARL has been developing programs to archive meteorological data fields, primarily for use in climate studies, but also for use with transport and dispersion model evaluation. One archive from the NMC Nested Grid Model was started in January 1989. This archive consists of 5 three-dimensional fields (U, V, and W wind components, specific humidity, and temperature) between 0.9823 sigma (~ 175 m) and 0.72101 sigma (~ 2790 m) and 6 surface fields (precipitation, exchange coefficient, heat flux, water vapor flux, pressure, and number of sigma surfaces within the mixed layer). These fields are archived on a 28 x 20 grid with a spatial resolution of 182.904 km at 60N latitude and a temporal resolution of 2 hours.

On September 1, 1990, a new NGM archive was initiated. The new archive has the same spatial (182.904 km at 60N) and temporal (2 hours) resolution as the original archive, but with a larger spatial domain, more vertical levels, and more surface fields. The 5 three-dimensional fields are now available between 0.9823 sigma (~ 175 m) and 0.43414 sigma (~ 6600 m). The additional surface fields are ice-covered water surfaces, snow coverage, surface height, mean sea level pressure, and convective precipitation. All fields are on a 33 X 28 grid covering all of the United States and southern Canada. Since the new archive retains all the information from the original archive while adding more fields and levels, it is planned to replace the original archive on January 1, 1991. The data from the new archive will greatly enhance transport and diffusion models by allowing more vertical transport and greater boundary layer parameterizations.

A second archive, which will be used exclusively for climate studies, will consist of 6-hourly global analyzed meteorological fields. The archived fields are from NMC's "Final" (FNL) Run, which is the last run in every forecast cycle (00 and 12 GMT) at NMC. This allows late arriving conventional and satellite data to be included in the analyses. FNL runs at 06 and 18 GMT provide analyses fields as well as 6-h subsequent forecast fields which are used in the initialization of subsequent forecast runs. Wind component (u, v, and w), temperature, relative humidity, and height fields on mandatory pressure levels are archived. The u-and v-component winds, temperature and height are on the 1000, 850, 700, 500, 400, 300, 250, 150, 100, 70 and 50 mb levels. The w-component fields are on the levels from 1000 to 100 mb. Relative humidity fields are on the levels from 1000 to 300 mb. Surface pressure and temperature, and mean sea level pressure are also archived. Both northern and

southern hemisphere data are archived on a 65 x 65 polar stereographic grid with spatial resolution of 381 km at 60° latitude. The data are packed in the same format as ARL's NGM-data archive so that computer programs may access the data in either archive with relative ease. Computer programs to create the archive and maintain it are also similar to simplify operations. The FNL global archive should become operational in 1991.

In order to manage the immense amount of data for these archives, ARL has recently installed an IBM RISC-6000 computer, with 16mbytes of memory, a 1.44Mbyte 3.5-inch diskette drive, a 355Mbyte fixed disk, a 2 gigabyte tape drive, a CD ROM drive and a 19-inch 1280 x 1024 pixel resolution color monitor with an IBM Color Graphics Display Adapter capable of displaying 256 colors from a 16.7 million color palette. The computer MIPS rating is 34.5 and its MFlop rating is 10.9, allowing it to perform at speeds near or equal to Mid-range Vector Machines and in some instances it has exceeded 50% of the speed of a CRAY Y-MP mainframe. The machine is an AIX (UNIX) based computer, with the capability of simulating a fast PC, allowing DOS based programs to be used. It comes LAN ready; that is, it is already setup to be integrated into a Token-ring or Ethernet network. Its physical dimensions are about those of an oversized PC. ARL will use the RISC-6000 in a Token-Ring LAN to access and archive meteorological data on a real time basis from the National Weather Service mainframes onto optical drives or tapes, giving laboratory scientists ready access to the latest data for ER responsibilities or to data for special archiving for climate studies.

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