United States Environmental Protection Agency
Research and Development

Environmental Sciences Research Laboratory
Research Triangle Park NC 27711

EPA-600/S3-84-092 Nov. 1984

EPA

Project Summary

Field Validation of Exposure Assessment Models

J.C. Doran, O.B. Abbey, J.W. Buck, D.W. Glover, T.W. Horst, R.N. Lee, and F.D. Lloyd

This report, in two volumes, describes work done to evaluate the Point, Area, and Line source model (PAL), a Gaussian diffusion code modified to account for dry deposition and settling (the modified model is designated PAL-DS). The first volume describes the experimental techniques employed to dispense, collect, and measure depositing (zinc sulfide) and nondepositing (sulfur hexafluoride) tracers. The measured concentrations of the tracers form a data set by which the PAL-DS model may be tested. These concentrations are given in tabular and graphic form for five downwind distances from the release point, ranging from 100 to 3200 m. Measurements of wind speed, direction and temperature at seven heights from 1 to 61 m were taken during the tracer releases as well as several parameters describing the turbulence characteristics. A discussion of particle size distributions of the depositing tracer is given, and the calibration and quality assurance procedures used for sample analysis are described. Two chlorocarbon tracers were also used in the tracer releases, but with little success. The first volume concludes with a discussion of the problems encountered with these tracers and some recommendations for possible solutions.

The second volume contains an analysis of the field data and an evaluation of four atmospheric dispersion models, PAL-DS and three similiar alternates. The four models are described, and an evaluation of the performance of each is given. The evaluation is based on an analysis of C_d/C_o, the ratio of the crosswind-integrated concentrations of a depositing and nondepositing tracer, respectively, at a height of 1.5 m. The PAL-DS model is found to overestimate this ratio; a corrected source depletion model appears to give significantly better results. A novel method of determining the effective deposition velocity of the depositing tracer, based on a surface depletion, approach is described. A discussion of model sensitivities, experimental design, and the effects of measurement errors on the model evaluation is also given. Experimental uncertainties may well affect the performances of the models, but it is doubtful that their relative performances would be significantly changed. Errors in describing the diffusion meteorology are likely to be more important in predicting depleted concentrations than errors introduced by the choice of a particular deposition model.

This Project Summary was developed by EPA's Environmental Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The basic aim of this work was to release and sample tracers in the atmosphere, to obtain data suitable for an evaluation of EPA is PAL model as modified for depositing pollutants, and to perform such an evaluation. An additional goal was to make some limited releases of organic tracers and evaluate their measurement accuracy under controlled field conditions.

The PAL model is a Gaussian plume diffusion code for point, area, and line sources which have been modified to account for dry deposition and settling. The resulting PAL-DS code uses diffusion-deposition algorithms that are based on analytical solutions of a gradient-transfer model for dry deposition of gaseous and suspended particulate pollutants from a plume.

In order to evaluate the PAL-DS model, three kinds of data are required: the distribution of some tracer subject to deposition to the surface, the distribution of some other tracer not subject to deposition, and the prevailing meteorology during the measurement periods. Zinc sulfide (ZnS) was chosen for the depositing tracer, while sulfur hexafluoride (SF_6) was used for the nondepositing tracer. Wind and temperature sensors mounted on several towers were used to assess the meteorological conditions during the tracer releases. Several organic tracers were also tried, but with little success.

The first volume provides a description of the experimental techniques employed to dispense, collect, and measure the tracers used for the releases. It gives additional information on the characterization of the particle size distributions for the particulate tracer, the types of supporting meteorological measurements obtained, and the calibration procedures used for the tracer and meteorolgical measurements. The report is specifically concerned with various aspects of quality assurance in the collection and analysis of the data. Finally, the report contains listings and figures describing the principal features of the measured tracer distributions and the winds and temperatures during the releases.

The second volume presents an analysis of the data that enables effective deposition velocities for the depositing tracer to be determined, and uses these and other estimates in an evaluation of the principal features of the PAL-DS model and three other models. It also presents a statistical summary of the performance of these models, in simulating the observed behavior, gives some suggestions for interpreting this behavior, and recommends possible additional measurements and modeling studies that would further clarify the behavior of depositing materials.

Experimental Procedures

The Hanford diffusion grid, where the tracer measurements were obtained, is located in a semiarid region of southeastern Washington on generally flat terrain. The vegetation consists primarily of desert grasses and 1 to 2 m high sagebrush.

Five sampling arcs, located at distances of 100, 200, 800, 1600, and 3200 m from the tracer release point, were used for tracer collection. A 122-m meteorological tower was located approximately 100m to the north of the release area. It contained wind speed, wind direction and temperature sensors at various elevations. These data were used to monitor conditions during tracer releases in an effort to ensure that material was released during periods with appropriate wind and stability conditions. Near-neutral to stable conditions were selected to maximize differences in concentrations of depositing and nondepositing tracers.

For subsequent, detailed analysis of the meteorology, data were collected at a second tower located in the center of the 1600-m arc. That tower was 61-m high, and was equipped with 3-component propeller anemometers and aspirated bead thermistors at seven heights. All anemometers were located on booms extending at least 2 tower diameters west (generally upwind) of the tower. Data from all sensors were recorded on magnetic tape approximately once every 2.3 s.

A 3-m tower was located about 25 m to the southwest of the 61-m tower, and held a 3-component sonic anemometer and fast-response platinum resistance thermometer on a boom extending from its top.

The ZnS was collected on membrane filters mounted 1.5 m above the surface. The vacuum pumps used to draw air through the filters were driven with gasoline engines, and flow through the filters was regulated by critical flow orifices inserted just downstream of each filter holder assembly. Filters were located at 2° increments on the 100-, 200- and 800-m arcs, and at 1° increments on the 1600- and 3200-m arcs. Each arc encompassed a sector of approximately 90°. The SF_6 tracer was sampled at intervals of 8° at the 100-m arc, 4° at the 200- and 800-m arcs, 2° at the 1600-m arc and 3° at the 3200-m arc. Multilayer bags were deployed at intervals of 12° at the 800-m and 3200-m arcs and 8° at the 1600-m arc. Some effort was also made to measure vertical profiles of the tracer concentrations, and two towers at the 1600-m arc were equipped with filters and pumps to a height of 25 m.

The ZnS particulate tracer was dispensed with an aerosol generator. The ZnS was mixed with a 1%, by weight, fluidizing agent. Prior to tracer release, the mixture was loaded into a hopper on the generator. Material from the hoppe was dropped, via a notched wheel, into blower assembly, which ejected th particles horizontally into the atmosphere During the release, the ZnS was contin uously stirred to ensure smooth feedin of the particles into the blower.

The SF_6 was dispensed from a 91-lite tank that had been previously filled from SF_6 cylinder to a moderate pressure. Th flow from the tank was regulated via needle valve and rotometer, and the SF was released through a length of poly ethylene tubing. Typical release rate were on the order of 0.3 g/s.

The organic tracers were release using a pressurized tank and generatin gun assembly. The gun consisted of ar outer aluminum tube, two ultrasoni nozzles, and a perforated tube behind th nozzles that provided a sheath of ai isolating the organic material from th outer tube.

All tracers were released from a heigh of 2 m. The separation between the SF and ZnS release points was less than 1 m, while the distance between the ZnS and organic tracer release points was about 5 m.

Concentrations of ZnS on the filters were determined by using a device developed at Hanford and known as a Rankin counter. Its essential elements consist of a weak plutonium source of alpha particles, which are used to induce fluorescence in the ZnS particles, a photomultiplier tube used to detect this fluorescence, and a scaler used to count light flashes.

The SF_6 and organic samples were analyzed by means of gas chromatography. Calibrations of these instruments were obtained using National Bureau of Standards (NBS) traceable standards. The background detection limit for SF_6 was approximately 15 parts per trillion (ppt), and for the organic tracers it was about 0.1 parts per billion (ppb). Levels below these values were assumed to be due to background signals alone, and were not included in the data analysis.

Mean wind speeds, directions and temperatures are given for each release period and for an equal period after the releases so that one may obtain an idea of the stationarity of the conditions. As might be expected under stable conditions with low wind speeds, shifts in speed and direction were common, and the decision on the time to release tracers was made partially on the basis of an educated guess.

Winds speeds from a three component sonic anemometer and temperatures from a fast-response platinum resistance probe were recorded during parts or all of six of the releases. From these data we determined values of the friction velocity, temperature flux, and the Monin-Obukhov length.

Information is given on the standard deviations of the horizontal and vertical wind direction fluctuations, determined from the propeller anemometers. For a steady wind direction, the horizontal standard deviation is useful for predictions of the lateral plume spread, while the vertical standard deviation may be related to the vertical plume spread.

The report contains a brief, narrative description of conditions under which each of the six tracer experiments was conducted. The prevailing meteorology during the release period, the performance of the sampling equipment and some general descriptions of the resulting tracer distributions are given for the experiments which occurred during May and June of 1983.

Model Evaluation

The dual-tracer field measurements have been used to evaluate four Gaussian plume-depletion models: 1) the commonly used source depletion model, 2) a modified source depletion model that accounts for the alteration of the vertical concentration profile by deposition, 3) the PAL-DS model, which is a diffusion-deposition model based on a constant eddy-diffusivity solution of the advection-diffusion equation, and 4) a mass-conserving version of the PAL-DS model. These models are briefly described, and the general characteristics of their predictions are discussed in relation to those of an exact model of plume depletion.

The output of the models is a three-dimensional field of tracer concentrations. Measuring such a field in its entirety is clearly impossible, and some compromise is required. Moreover, the model output depends on a number of factors, which may be roughly divided into two classes: those describing the diffusion meteorology and those describing the deposition. In reality the two sets of factors are related, but the diffusion aspects of various models have been evaluated extensively in a host of studies. There appears to be little point in emphasizing such analyses for our limited data set; instead, we focus on the deposition part of the model. To evaluate the model's performance, we assume that the diffusion meteorology is known or can be determined. What remains, then, is to evaluate how well the model describes the depletion in the plume arising from deposition and settling. As noted earlier, we chose to employ a dual tracer technique for this exercise. The nondepositing tracer was SF_6, while ZnS was the depositing tracer. Differences in SF_6 and ZnS concentrations may be assumed to arise from the removal of depositing tracer at the surface, and the model description of this process may thereby be evaluated. Thus, the basic quantity to be discussed is the ratio C_d/C_o, where C_d is the crosswind-integrated concentration of depositing tracer 1.5 m above the surface and C_o is a similar crosswind-integrated concentration of non-depositing tracer. In practice it was most convenient to measure concentrations of both tracers at some height close to the surface (1.5 m), where C_d-C_o is largest, rather than over an extended vertical extent.

The predictions of four models were evaluated. Comparisons of the predicted and measured values of C_d/C_o were made. The calculated ratios of C_d/C_o were determined by using the effective deposition velocities in each of the four models, for all six dual-tracer releases. The observed ratios are those actually measured in the field tests. The PAL-DS model showed the largest differences between observed and calculated values, while the corrected source depletion model shows the best agreement. The uncorrected source depletion model distributes the effect of deposition uniformly through the vertical extent of the plume, rather than preferentially depleting the plume at ground level, and thus overestimates the near-surface concentration ratio. Much better results are given by the corrected source depletion model, which accounts for the change in the vertical distribution caused by deposition.

Conclusions and Recommendations

The PAL-DS model was found to overestimate consistently the amount of depositing pollutant at a height of 1.5 m. A corrected version of this model, which incorporates a modification that ensures conservation of mass, performed better, while a corrected source depletion model gave the best results of the four models tested. In all cases uncertainties in describing the diffusion meteorology are apt to be more important for estimating depleted air concentrations than differences arising from the choice of a particular deposition model. However, of the four models tested, the use of the corrected source depletion model appears to offer the best chance of avoiding systematic errors in the description of plume loss arising from deposition.

Because a number of uncertainties in the tracer concentration measurements and their analyses may have adversely affected the model evaluations, statistical comparisons of model performance should be viewed with some caution. However, the relative performances of the four models seem unlikely to be seriously affected by these factors.

Three additional tasks are suggested that would provide greatly increased confidence in model evaluations such as those just described and could result in better quantitative comparisions of models with each other or with theory. While relatively simple to state, each task is a major research effort in itself.

The first task is the development of a tracer generator capable of producing mono-dispersed or nearly mono-dispersed particles in the size range 1-5 um diameter. The generator should be able to produce a quantity of material sufficient for detection at a range of 10 km or more. The tracer itself should be easily collected and analyzed. Such a tracer's size distribution could be more easily determined and non-isokinetic sampling effects could be estimated with better accuracy. Sample loss close to the source caused by the preferential depletion of larger size particles would be lessened, and the range of meteorological conditions in which the surface depletion method could be profitably used to determine deposition velocities would be increased.

The second task is a rigorous test of the surface depletion model of dry deposition, using this newly developed tracer technique. This task would involve a direct determination of the deposition velocity of a depositing tracer, e.g., by collecting material actually deposited on the ground, and the measurement of airborne concentrations of the depositing material close to the surface at a number of downwind arcs. These measurements could be done at relatively short distances from the tracer release point, on the order of 1 km or less.

The third task would be a more extensive evaluation of models such as the PAL-DS or corrected source depletion model. In particular, the distance to which concentration measurements are made should be increased to 10 km or more, in order to increase the range of values of plume loss that the models are to simulate. If a tracer generating technique such as that described above is used, substantial improvements in model evaluations should be possible.

J. C. Doran, O. B. Abbey, J. W. Buck, D. W. Glover, T. W. Horst, R. N. Lee, and F. D. Lloyd are with Pacific Northwest Laboratory, Richland, WA 99352.
***Jack Shreffler** is the EPA Project Officer (see below).*
The complete report consists of two volumes, entitled "Field Validation of Exposure Assessment Models:"
"Volume 1. Data," (Order No. PB 85-107 209; Cost: $17.50)
"Volume 2. Analysis," (Order No. PB 85-107 217; Cost: $10.00)
The above reports will be available only from: (costs subject to change)
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
The EPA Project Officer can be contacted at:
Environmental Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

☆ U S GOVERNMENT PRINTING OFFICE, 1984 — 559-016/7844

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

BULK RATE
POSTAGE & FEES PA
EPA
PERMIT No. G-35

Official Business
Penalty for Private Use $300