702717

PREPRINT UCRL- 76170 Rev. 2

Lawrence Livermore Laboratory

ADPIC - A THREE-DIMENSIONAL PARTICLE-IN-CELL MODEL FOR THE DISPERSAL OF ATMOSPHERIC POLLUTANTS AND ITS COMPARISON TO REGIONAL TRACER STUDIES

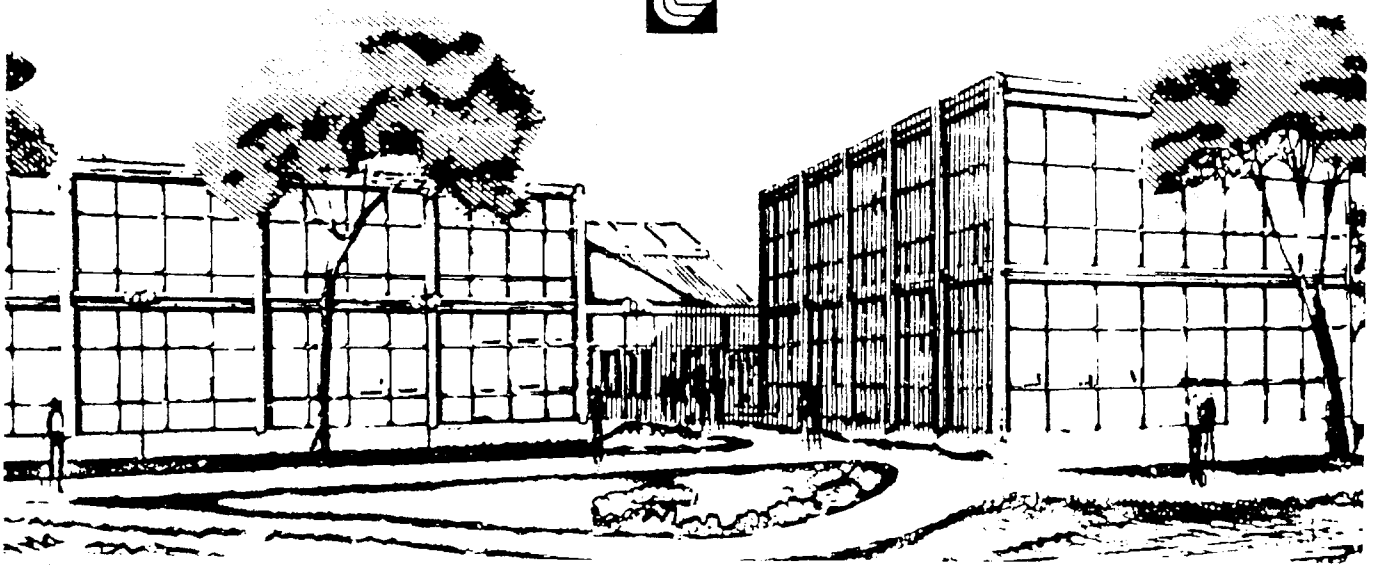
Rolf Lange

October 1976

REPOSITORY LLNL
COLLECTION TID Reports Library
BOX No. 174 258 (Acc. No.)
FOLDER

This paper was prepared for submission to *Journal of Applied Meteorology*

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.



0023840

ADPIC - A THREE-DIMENSIONAL PARTICLE-IN-CELL MODEL FOR THE DISPERSAL OF ATMOSPHERIC POLLUTANTS AND ITS COMPARISON TO REGIONAL TRACER STUDIES

Rolf Lange
Lawrence Livermore Laboratory, University of California
Livermore, CA 94550

November 1976

ABSTRACT

A hybrid Lagrangian-Eulerian atmospheric transport-diffusion model was developed to calculate the three-dimensional distribution of atmospheric pollutants in transient-region flow fields. This Atmospheric Diffusion Particle-in-Cell (ADPIC) code was validated against several existing closed-form analytical solutions including a puff release in steady, unidirectional shear flow, and a puff release with scale-dependent horizontal and vertical eddy diffusion coefficients. These tests showed that the ADPIC results were within a 5 percent error when compared to the analytic solutions. Regional tracer studies at the National Reactor Test Station Idaho Falls, Idaho, and at the Savannah River Laboratory, Aiken, South Carolina, were also used to compare the code against field measurements.

0023841

1. INTRODUCTION

The Atmospheric Diffusion Particle-in-Cell (ADPIC) code is a numerical, three-dimensional, Cartesian, particle-diffusion code capable of calculating the time-dependent distribution of air pollutants under many conditions. These conditions include strongly distorted advection wind fields, calm conditions, space-variable surface roughness, wet and dry deposition, radioactive decay, and space- and time-variable diffusion parameters.

Basically, the code solves the three-dimensional advection-diffusion equation in its flux conservative form (pseudovelocity technique) for a *given* non-divergent advection field by finite difference approximations in Cartesian coördinates. The method is based on the particle-in-cell technique with the pollutant concentration represented by Lagrangian-marker particles inside a fixed Eulerian grid (Welch, Harlow, Shannon and Daly, 1965; Amsden, 1966; Shlarew, Fabrik and Prager, 1971; Lange, 1973). Most air pollution scenarios involve time- and space-varying advection fields (shear) and diffusion parameters. They involve topography, precipitation, and gravitational effects for a variety of active or inert source and are inherently three-dimensional in nature. ADPIC was developed to model these aspects of pollutant dispersal over short or long times for any specified source term with the exception, for the present, of photochemistry.

With the development of the three-dimensional non-divergent (mass-conservative) windfield model MATHEW (Sherman, 1975), which is used to provide the full three-dimensional space- and time-varying advection field to ADPIC, pollutant dispersion studies of any desired complexity can be undertaken.

0023842

ADPIC has undergone extensive validation tests against closed analytic solutions and regional tracer studies (Lange, 1973) and compares to within a 5% error against selected analytic solutions. Agreement is remarkably consistent against methyl iodine tracer studies at NRTS, Idaho Falls, Idaho and ^{41}Ar plumes at Savannah River Laboratory, Aiken, South Carolina. ADPIC concentrations are 60% of the time within a factor of 2 and 95% of the time within an order of magnitude of measurements without any *tuning* of the model to any specific site, tracer scenario, or tracer material. As such, these yet partial validation results can be viewed as an emerging indicator of the degree of accuracy with which the ADPIC-MATHEW package can compute complex regional pollutant concentration and deposition distributions.

2. DESCRIPTION OF ADPIC

The pseudo-velocity method consists of the following: given the non-linear transport-diffusion equation

$$\frac{\partial \chi}{\partial t} + \overline{U}_A \cdot \overline{\nabla}\chi = \overline{\nabla} \cdot (K\overline{\nabla}\chi) \quad , \tag{1}$$

where χ is a scalar concentration, K is the diffusion coefficient and $\overline{U}_A$ the (given) non-divergent advection velocity field, we can, under the assumption of incompressibility, replace the $\overline{U}_A \cdot \overline{\nabla}\chi$ term by $\overline{\nabla} \cdot (\chi U_A)$, Upon combining the two divergence terms, we can rewrite Eq. (1) in its flux conservative (pseudo-velocity) form

$$\frac{\partial \chi}{\partial t} + \overline{\nabla} \cdot \left[\chi(U_A - \frac{K}{\chi}\overline{\nabla}\chi)\right] = \frac{\partial \chi}{\partial t} + \overline{\nabla} \cdot (\chi \overline{U}_P) = 0 \quad , \tag{2}$$

where $\overline{U}_P \equiv \overline{U}_A - \frac{K}{\chi}\overline{\nabla}\chi$ is defined as pseudo-transport velocity. The advection field $\vec{U}_A$ is generally supplied by a non-divergent three-dimensional wind field model like MATHEW (Sherman, 1975). The term $- K \frac{\overline{\nabla}\chi}{\chi}$ is a diffusivity velocity $\overline{U}_D$.

The grid mesh of the code is represented by an Eulerian grid consisting of three-dimensional rectangular cells of uniform size. The concentrations χ are defined at the centers of the cells and the velocities $\overline{U}_A$, $\overline{U}_P$ and $\overline{U}_D = - \frac{K}{\chi}\nabla\chi$ are defined at the cell corners. The locations of the particles, which represent the pollutant cloud are defined by their individual Lagrangian coordinates within the Eulerian fixed grid.

A time cycle of the code is divided into an Eulerian step and a Lagrangian step and proceeds as follows:

- Eulerian Step: The concentrations χ, given for each cell at the beginning of the cycle, are used to calculate the diffusivity velocities $U_D = - \frac{K}{\chi}\overline{\nabla}\chi$ which are then added to the wind advection velocities $\overline{U}_A$ to yield a pseudo-velocity U_p for each cell corner.
- Lagrangian Step: Each marker particle contained in a given cell is transported for one time step ΔT with a velocity $\overline{U}$, which is computed from the pseudo-velocities $\overline{U}_p$ at the corners of the cell by a volume weighting scheme. The new particle coordinate $\overline{R}_{T+\Delta T}$ is obtained from the old coordinate $\overline{R}_T$ by a forward differencing scheme

$$\overline{R}_{T+\Delta T} = \overline{R}_T + \overline{U} \cdot \Delta T \tag{3}$$

Finally, a new concentration distribution χ is calculated from the new particle positions, thus ending the cycle.

The Eulerian-Lagrangian particle-in-cell method has two chief advantages over purely Eulerian schemes. First, the fictitious Eulerian numerical diffusion is eliminated because the pollutant concentration is transported and diffused along the Lagrangian trajectories of the marker particles. Second, each marker particle can be tagged with its coordinates, age since generation, mass, activity, species and size, which greatly facilitates the computation of wet and dry deposition, radioactive decay, particle size distributions, radiation dose, and reaction rates of a pollutant.

Interpolation and truncation errors inherent in the finite difference algorithms remain, of course, and must be dealt with by the choice of the time step and cell size.

ADPIC uses staggered grids in which the velocities U and diffusivities K are defined at the cell corners while the concentrations χ are defined at cell centers. This has the following two important advantages over non-staggered grids.

The finite difference algorithm for the diffusion velocity in ADPIC, reduced to one dimension, is

$$U_{D_{i+1/2}} = - \frac{K_{i+1/2}}{\Delta X} \cdot \frac{(\chi_{i+1} - \chi_i)}{\frac{1}{2}(\chi_{i+1} + \chi_i)} \tag{4}$$

where $U_{D_{i+1/2}}$ and $K_{i+1/2}$ are the diffusion velocity and the diffusivity at the cell corners i+1/2, and χ_{i+1} and χ_i are the concentrations at the i+1

and i cell centers and ΔX is the cell size. For non-staggered grids this expression takes the form

$$U_{D_i} = - \frac{K_i}{2\Delta X} \frac{(\chi_{i+1} - \chi_{i-1})}{\chi_i} \quad . \tag{5}$$

The advantages of Eq. (4) over (5) are that the diffusion velocity U_D does not become infinite when the concentrations in the denominator go to zero, and that only one layer of cells around the outside of the grid is required to specify the boundary conditions.

When the expression for the diffusivity velocity U_D, Eq. (4), is expanded in a Taylor series and a Gaussian concentration distribution is chosen and substituted for χ into this series expansion, one obtains an expression for the truncation error of U_D in form of a ratio of the ADPIC diffusivity velocity U_D divided by the exact differential expression for the diffusivity velocity $U_D = - K \frac{\partial \chi}{\partial x}$. In one dimension and retaining only the highest error term, this ratio is

$$\frac{U_D(\text{ADPIC})}{U_D(\text{exact})} = 1 - \left(\frac{\Delta X}{2\sigma_x}\right)^2 \tag{6}$$

where Δx is the grid cell size and σ_x is the standard deviation of the assumed Gaussian concentration distribution. Equation (6) indicates that by choosing enough cells to resolve a pollutant distribution, i.e., $\sigma_x \geq 2\Delta x$, the truncation error can be made as small as desired.

Due to the part-Eulerian, part-Lagrangian nature of ADPIC, the boundary conditions break up into one set of conditions imposed on the Eulerian velocity field and one set imposed on the Lagrangian particles. Both sets must be consistent with each other.

The two basic boundary conditions imposed on the pseudo-velocity field in ADPIC $\vec{U}_p = \vec{U}_A + \vec{U}_D$ are constant mass flux, $(\chi\overline{U}_p)$ = constant, corresponding to inflow and outflow of particles, and zero mass flux $(\chi\overline{U}_p) = 0$, corresponding to reflection of particles from the boundary. There are intermediate cases as, for example, deposition of particles at the topography, in which case a deposition velocity is specified. In the kind of studies that ADPIC has so far been used for, the concentration field is smooth enough by the time it reaches the outflow boundary that the outflow boundary condition can be specified by postulating a constant flux of particles through the boundary grid cell layer.

The particle boundary conditions are very simple. If a particle has been found to have left the grid during a cycle, it is either annihilated or counted as deposited or is reflected, according to the type of boundary specified.

ADPIC requires large amounts of core storage space. Most of the usable large core memory (about 340 000 decimal words) of a CDC 7600 computer is needed to run ADPIC for a regional study. A rough upper limit size for such a problem would be 25 000 cells (50 x 50 in the horizontal x 10 in the vertical) and 30 000 particles. In this mode the computational speed of ADPIC is about 100 times faster than real-time.

0023847

3. VERIFICATION OF ADPIC AGAINST ANALYTICAL SOLUTIONS

Selected analytic solutions to the diffusion-advection Eq. (1) were chosen in order to verify the ADPIC code. Because of the intractability of this equation analytic solutions exist for only rather simple, linearized cases with Gaussian pollutant distributions. Table 1 summarizes the cases chosen for the basic verification of ADPIC. Overall, ADPIC results agreed with the closed Gaussian solutions to within a 5 percent error (Lange, 1973). The time and spacial scales and other parameters, like source configuration and diffusion parameters, were chosen in such a way as to make the verification cases compatible with scale relations in the real atmosphere. On this basis the 5 percent maximum error between ADPIC and analytic solutions holds over regional scales of many hours and hundreds of kilometres. There is no indication that this error will increase if the cases described in Table 1 were run for even much longer periods or larger distances.

While these simple test cases in no way represent a full verification of the model, importance of these results are that the ADPIC code represents a reasonably accurate calculational framework for attacking regional transport-diffusion problems for transient regional flow fields in multidimensional space. The quality of the ADPIC solutions for the real atmosphere, therefore, is governed by our knowledge of the temporal-spatial regional flow fields and the spatial distribution and time dependency of the eddy-diffusion processes, and source terms.

0023848

4. VALIDATION OF ADPIC AGAINST A REGIONAL TRACER STUDY AT THE IDAHO FALLS NRTS SITE

For the past several years, the National Oceanic and Atmospheric Administration has performed regional tracer tests at the Idaho Falls National Reactor Test Station (NRTS). The NRTS staff provided both the meteorological and source-term information for one of their methyl iodine releases. That test consisted of a 3-h injection of methyl iodine with ^{131}I into a transient regional flow field. Meteorological properties were documented by 17 meteorological towers as well as by upper level wind measurements and indicated a neutral Pasquill C category. 36 volume field samplers were arranged in four arcs at various distances downwind form the source.

The regional flow field was calculated by the LLL three-dimensional mass-conserving windfield code MATHEW (Sherman, 1975). ADPIC simulated the time history of the passage of the cloud over each of the samplers while also calculating the total spatial-temporal distribution of the pollutant. The details of the ADPIC problem setup and a summary of the results are included in Table 2.

As an aid to interpreting the results, Fig. 1 shows an illustration of the complex topography of the Idaho Falls region and the general outline of the plume as it was transported downwind from its source. The vertical scale is strongly enhanced.

Fig. 2 shows the horizontal projection of the Lagrangian marker particles representing the cloud onto the horizontal plane and the sampler arcs at 3 h. Embroidery along the left side of the pollutant cloud is caused by topographical effects.

ADPIC samples concentration by counting those Lagrangian particles that pass through a sampler volume. Such a simulated ADPIC surface-air concentration history at sampler A-3 is shown in Fig. 3 and is compared in terms of its breadth with the actual passage time of the plume as documented by field measurements. Unfortunately the field measurements gave only total time integrated concentrations and time of passage. Therefore comparison with ADPIC was only possible on the basis of the total area under the ADPIC sampler curves like the one in Fig. 3.

Figure 4 shows the time integrated concentration of the samplers along arc C as a function of crosswind distance for both ADPIC and field measurements. These integrated concentrations are also compared with the results obtained by solutions using a Gaussian plume equation for the stability category C. The Gaussian plume result in Fig. 4 was overlayed on what was considered to be the main branch of the ^{131}I plume and was not based on the wind speed and direction at the source. If the Gaussian plume had been based on the wind at the source, it would have partially missed the sampler arc C in Fig. 4. Although the Gaussian solution matches the peak concentration at what might be construed as the plume centerline, it is too narrow and the second peak cannot be accounted for. The second peak is a result of temporal changes in the regional flow field and an effect of the topography.

Figure 5 is a scatter diagram comparing the ADPIC time integrated ^{131}I surface air concentrations with measured values for all 36 samplers. The principal sources of error result from the prescription of the regional flow field, the prescription of eddy diffusion coefficients as derived

from bulk meteorological parameters, and the sensitivity of the surface-air concentration to the representation of topography in the MATHEW and ADPIC codes.

5. COMPARISON OF ADPIC AGAINST THREE ^{41}Ar PLUMES AT SAVANNAH RIVER LABORATORY, SOUTH CAROLINA

During Spring 1974, three daily 6-h exercises were initiated to compare ADPIC against data from three ^{41}Ar plumes at the Du Pont Savannah River Plant (SRP) in Aiken, South Carolina. Because of their typical difference in synoptic condition, the second and third dat test scenarios were chosen as detailed validation experiments for ADPIC. Test 2 had mostly light 1 to 3 m/s winds varying over more than 180° during the 6-h test while Test 3 had rather steady 1 to 4 m/s winds varying over less than 90° during the test. Both tests started at 8:00 a.m. Eastern Daylight Time with approximately an F-Pasquill stability and a temperature inversion at a height of about 140 m breaking up an hour or so later. Both tests ended at 2:00 p.m. EDT with approximately a C-Pasquill stability.

Figure 11 shows the SRP site with the C, K, and P reactors, which are the sources for the three ^{41}Ar plumes, each having a stack height of 60 m. The topography of the site and its surroundings varies over about 75 m, mostly because of the Savannah River bed; it is alternately open grass land, crops, and young pine forest. In the models topography proturdes in rectangular building block fashion into the grid from below.

The meteorological data for wind speed, direction, and their turbulent intensities (sigmas), were taken at 5-s intervals at a height of 60 m from two site towers in the P and H area, and at several heights up to 360 m from the WJBF-TV tower located 30 km northwest from the site center. In addition to providing the vertical variation of the windfield, the TV tower also provided the vertical temperature profile.

The measurements of ^{41}Ar concentrations from the three reactor plumes were obtained by looking at the peak-γ window of the radioactive ^{41}Ar with sodium iodide crystals. For Test 2, measurements were taken by two detector-equipped cars at a 2-m height at 20 different 10-min sampling stops. To track the plumes the sampling stops were made anywhere within about a 25 km radius from the sources as permitted by the road network. For Test 3, in addition to 22 measurements from the two cars, a detector-equipped helicopter from EG&G, Inc., Las Vegas, Nevada, tracked the plumes at heights of 150 and 300 m above topography. The helicopter flew a total of 19 more or less straight-line sampling passes (at speeds of about 50 m/s) each of which lasted approximately 3 to 7 min and collected data at 6-s intervals.

The ADPIC validation problem setup for the Savannah River plumes and comparison of results with measured data is shown in Table 3. The three-dimensional mass-consistent advection field $\vec{U}_A$ was provided by the MATHEW (Sherman, 1975) code in 15-min-averaged data sets using interpolated data from the three meteorological towers. The three plume sources were modeled by continuous generation of ADPIC particles, each representing a fixed amount of activity and possessing an "age" label to allow for radioactive decay calculation according to the ^{41}Ar decay constant of $1.04 \times 10^{-4}\ s^{-1}$. Typically, at any given time about 12 000 particles were present in the grid to represent the plumes.

The horizontal diffusion coefficients K_H were obtained directly from the rms wind direction fluctuations σ_θ as measured by the TV-tower instruments as a function of height. The relationship used is

$$K_H = d/dt(\sigma_H^2) \qquad \text{with} \qquad \sigma_H = \sigma_\theta |\vec{r}|^{0.91} \quad , \tag{7}$$

where σ_H is the standard deviation of the plume width, $\vec{r}$ is the distance from the source, and d/dt is the time derivative. The vertical diffusion coefficient K_z was set to increase linearly with height according to $K_z = (K_{zM}/H)z$, where K_{zM} is K at the top of the mixing layer, H is the height of the mixing layer, and z is the height above the surface. Typical values for K_{zM} for the stable to slightly unstable conditions encountered were picked from SRP statistical data (Crawford, 1974), and varied from 1 to 25 m^2/s.

Sampling is done in ADPIC by counting particles, each representing a certain amount of activity. For comparison with field data, ADPIC simulated the sampling at the fixed car locations and also simulated a moving detector to model five of the helicopter flights. Figure 7 shows the ADPIC particle simulation of the C, P, and K plumes together with one of the helicopter runs. Figure 8 is a typical example of data obtained by real and ADPIC helicopters.

Figure 9 shows the results of the ADPIC comparison with measurements for cars (Test 2 and Test 3) and also for helicopters (Test 3). Shown are the relative air concentrations for 40 surface samplers and 9 helicopter flights. As already indicated in Table 3, about 60% of the time the ^{41}Ar plume concentrations computed were within a factor of 2 of measured, while 98% of

the time they agreed within an order of magnitude. In more detail, ADPIC agreed better with the car data of Test 3 than of Test 2. This is a result of the major difference between the two tests in the most sensitive parameter, namely the high variability of wind direction during Test 2 in contrast to the much steadier Test 3 conditions. The enormous sensitivity of the regional air concentrations to wind direction for the case of point sources is illustrated by Figs. 10 through 13.

Figures 10 and 11 show the ADPIC plumes for the C, P, and K reactors for Test 2 at 12:00 and 13:00 EDT. In one hour, the winds have swung from easterly to southerly to westerly, resulting in the breakup of the plumes of Fig. 10. This shift literally paints a 180° sector before new steadier winds begin to establish new plumes as shown in Fig. 11. Figures 12 and 13 represent the corresponding ADPIC isopleths at a height of 2 m together with the detector car locations at those times. The choppiness of the contours is caused by topography. Keeping in mind the scale of the figures an appreciation can be gained for the difficulty of plume air concentration data collection (plume chasing) on the regional scale. In addition to the gross effects of the wind direction variability discussed, Figures 10 through 13 also show the local difference in the advection field as depicted by the difference in direction of the three simultaneous plumes.

On the regional scale, data collected by one moving detector (moving fast compared with wind speeds, such as the helicopter used in Test 3) are more conclusive than even a large number of fixed surface detectors at least for variable winds. Figure 8, showing concentration versus time for a single helicopter pass, illustrates the point: one pass of the helicopter

sampler yields a snapshot of the plume cross sections showing centerline direction, maximum concentration and plume width.

Comparison of the field helicopter trace with the ADPIC model helicopter allows separation of model errors caused by the advection field (offset of peaks) from errors caused by diffusion parameters (plume width and peak concentrations). Figure 8 shows that the advection field used in ADPIC was in error for the K plume while it was correct for the P plume. The reason is that the mass-consistent advection field had meteorological input data at the P reactor while it had to rely on an interpolated value at the K reactor. In addition, the diffusion parameters used in ADPIC appear to diffuse the plume somewhat too slowly.

Figure 9 shows that 89% of the time (8 out of 9 peaks) the ADPIC helicopter results were within a factor of 4 of the measured EG&G helicopter data. This is in better agreement than for the cars for the same Test 3 because peak concentrations were compared for the helicopters, thus bypassing the errors caused by advection. The reason for the very low results of ADPIC for the 9th helicopter run is that one of the EG&G helicopter passes was nearly parallel to the K plume. Because the direction of the modeled K plume was off by a few degrees the ADPIC model helicopter missed it, thus reintroducing the importance of advection errors for passes at small grazing angles to the plume.

6. CONCLUSIONS

ADPIC was developed to study the pollutant dispersal and deposition on the regional scale from a variety of sources and for given advection fields. Of special interest are those cases for which source and terrain conditions are complex and the behavior of the atmosphere is nonuniform and nonsteady. For such cases the advection field can be provided in mass-conservative form from interpolated meteorological data by a mass-consistent windfield code such as MATHEW (Sherman, 1975). ADPIC computes the time-varying three-dimensional concentration field of inert as well as radioactive pollutants and can treat rainout, dry deposition, and inversion layers. A chief advantage of the particle-in-cell method is the lack of numerical diffusion errors present in other methods, and the capability to label the Lagrangian particles with various properties like mass, activity, size, time, etc.

The code was validated against a number of closed Gaussian solutions to the diffusion-advection equation including simple wind shear and scale-dependent diffusion, and was found to be accurate to within 5% of such solutions.

Regional tracer studies using ^{131}I at Idaho Falls and ^{41}Ar plumes at Savannah River Laboratory were used to validate ADPIC against regional field data using fixed high-volume samplers, γ-detector-equipped cars, and helicopters. Without *tuning* the model to any given regional site, type of source, or sampling method there appeared to emerge a uniformity in the accuracy in which ADPIC could model regional scenarios of pollutant dis-

0023856

persal as indicated by Figs. 5 and 9. Typically, 60% of the time ADPIC was within a factor of 2 of field data while 96% of the time it agreed to within an order of magnitude.

For modeling plumes on the regional scale the chief modeling errors in ADPIC, in decreasing order of importance, seemed to be wind direction, topography, diffusion parameters, source strength, and wind speed.

ACKNOWLEDGMENTS

I would like to thank Leonard Lawson for programming ADPIC and for organizing efficiently the enormously large data files necessary to run ADPIC with regional three-dimensional windfields.

This work was performed under the auspices of the U. S. Energy Research & Development Administration, under contract No. 7405-Eng-48, and supported in part by the National Science Foundation.

0023857

REFERENCES

Amsden, A. A., 1966: The particle-in-cell method for the calculation of the dynamics of compressible fluids. Los Alamos Scientific Laboratory, Report LA-3466.

Crawford, T. V., 1974: Progress report dose-to-man program FY-1973. E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, S. C. 29801.

Lange, R., 1973: A three-dimensional computer code for the study of pollutant dispersal and deposition under complex conditions. Lawrence Livermore Laboratory Report UCRL-51462.

Sklarew, R. C., A. J. Fabrik, and J. E. Prager, 1971: A particle-in-cell method for numerical solution of the atmospheric diffusion equation, and application to air pollution problems. Systems, Science and Software, La Jolla, Ca., Report 3SR-844.

Sherman, C. A., 1975: A mass consistent model for wind fields over complex terrain. Lawrence Livermore Laboratory Report UCRL-76171.

Welch, J. E., F. H. Harlow, J. P. Shannon, and B.J. Daly, 1965: The MAC method. Los Alamos Scientific Laboratory Report LA-3425.

0023858

TABLE 1. ADPIC verification against closed Gaussian solutions.

Case	Description
1	Instantaneous source, constant-K diffusion
2	Instantaneous source, scale-dependent $K(t)$ diffusion
3	Instantaneous source, constant-K diffusion in simple vertical speed shear $U = U(z)$, $V = W = 0$
4	Continuous source, constant-K diffusion (calm condition)
5	Continuous source, constant-K diffusion, advection $U = 2$ m/s
6	Continuous source, constant-K diffusion, advection $U = 10$ m/s

0023859

TABLE 2. Description of ADPIC simulation of field tracer study at NRTS, Idaho Falls.

Problem setup:

Number of grid cells: 16 x 24 x 24 = 9216

Vertical cell size = 50 m

Horizontal cell size = 4300 m

Stability category: Pasquill C

Source release rate = 0.379 mCi/s for 3 h. At 0.25 mCi/particles, this corresponds to 14,720 particles total.

Deposition velocity = 0.1 cm/s

Comparison between ADPIC and field-sampler results:

Agreement within factor of:	2	5	10
Fraction of total samples $\left(\frac{\text{ADPIC samplers}}{\text{Field samplers}}\right)$	0.44	0.81	0.94

TABLE 3. Description of ADPIC simulation of three ^{41}Ar plumes at SRP, South Carolina.

Problem setup:

Number of grid cells: 40 x 40 x 14 = 22400

Vertical cell size: 25 m

Horizontal cell size: day 2, 500 m; day 3, 1000 m

Atmospheric stability: Pasquill F through B

Source particles: 3 continuous sources with total release rate of 3 particles per second, corresponding to approximately 65,000 ADPIC particles over a six hour release period.

Comparison between ADPIC and measured results for both experiments:

Agreement within factor of:	2	5	10
Fraction of total samplers $\left(\frac{\text{ADPIC samplers}}{\text{Field samplers}}\right)$	0.61	0.92	0.98

0023861

FIGURE CAPTIONS

FIGURE 1. Idaho Falls topography and plume outline.

FIGURE 2. ADPIC particles representing the Idaho Falls plume after 3 h. (end of release time).

FIGURE 3. Activity vs. time for simulated ADPIC sampler A-3. Idaho Falls.

FIGURE 4. Time integrated activity for samplers on arc C. Idaho Falls.

FIGURE 5. Measured and computed time integrated ^{131}I surface air concentrations for 36 samplers at Idaho Falls.

FIGURE 6. The Savannah River Plant site (SRP).

FIGURE 7. Simulated helicopter flight path #838 and C, P, and K plumes as represented by ADPIC particles.

FIGURE 8. Helicopter flight #838, ADPIC and measured concentrations vs. time.

FIGURE 9. Measured and computed relative concentrations for three ^{41}Ar plumes at 49 samplers at SRP.

FIGURE 10. C, K, and P plumes for Test 2 at 12:00 EDT as modeled by ADPIC.

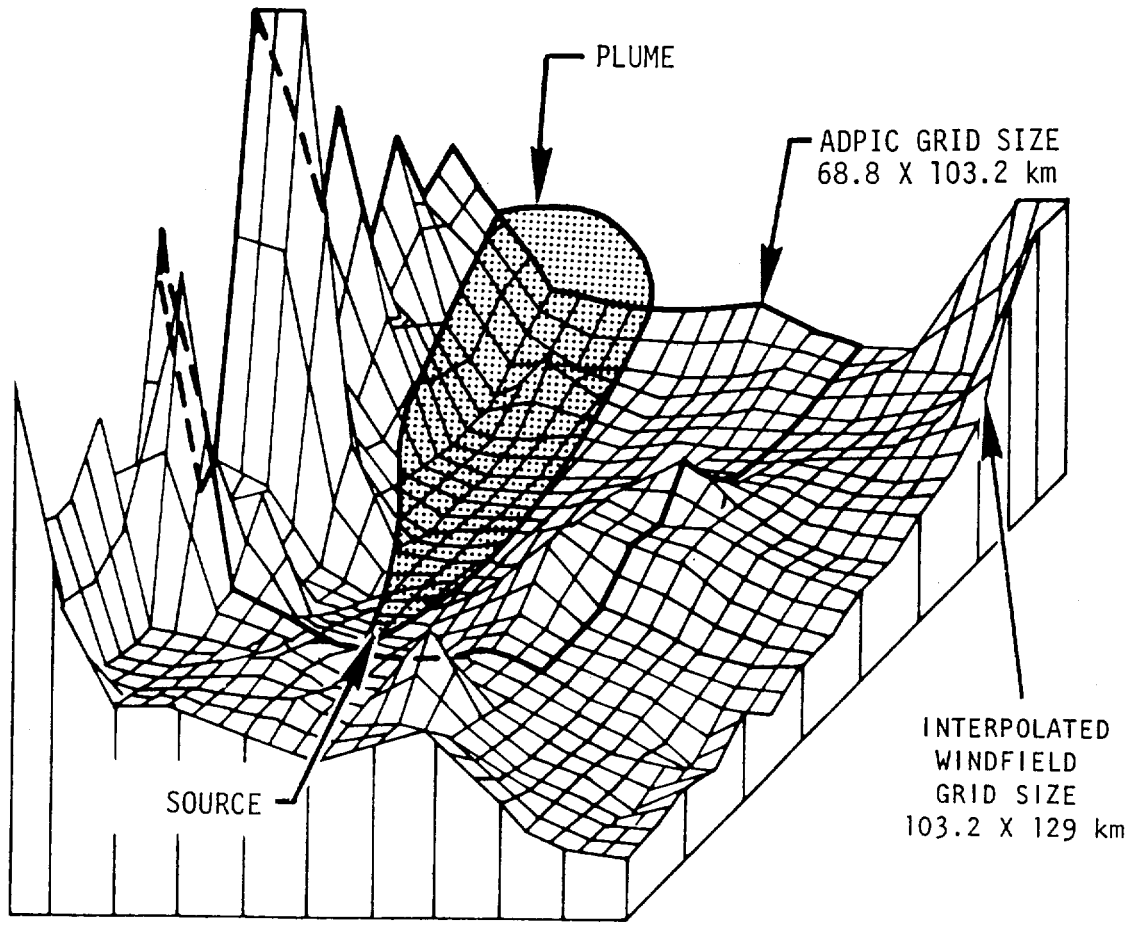
FIGURE 11. C, K, and P plumes for Test 2 at 13:00 EDT as modeled by ADPIC.

FIGURE 12. C, K, and P plume activity isopleths from ADPIC for Test 2, 12:00 EDT.

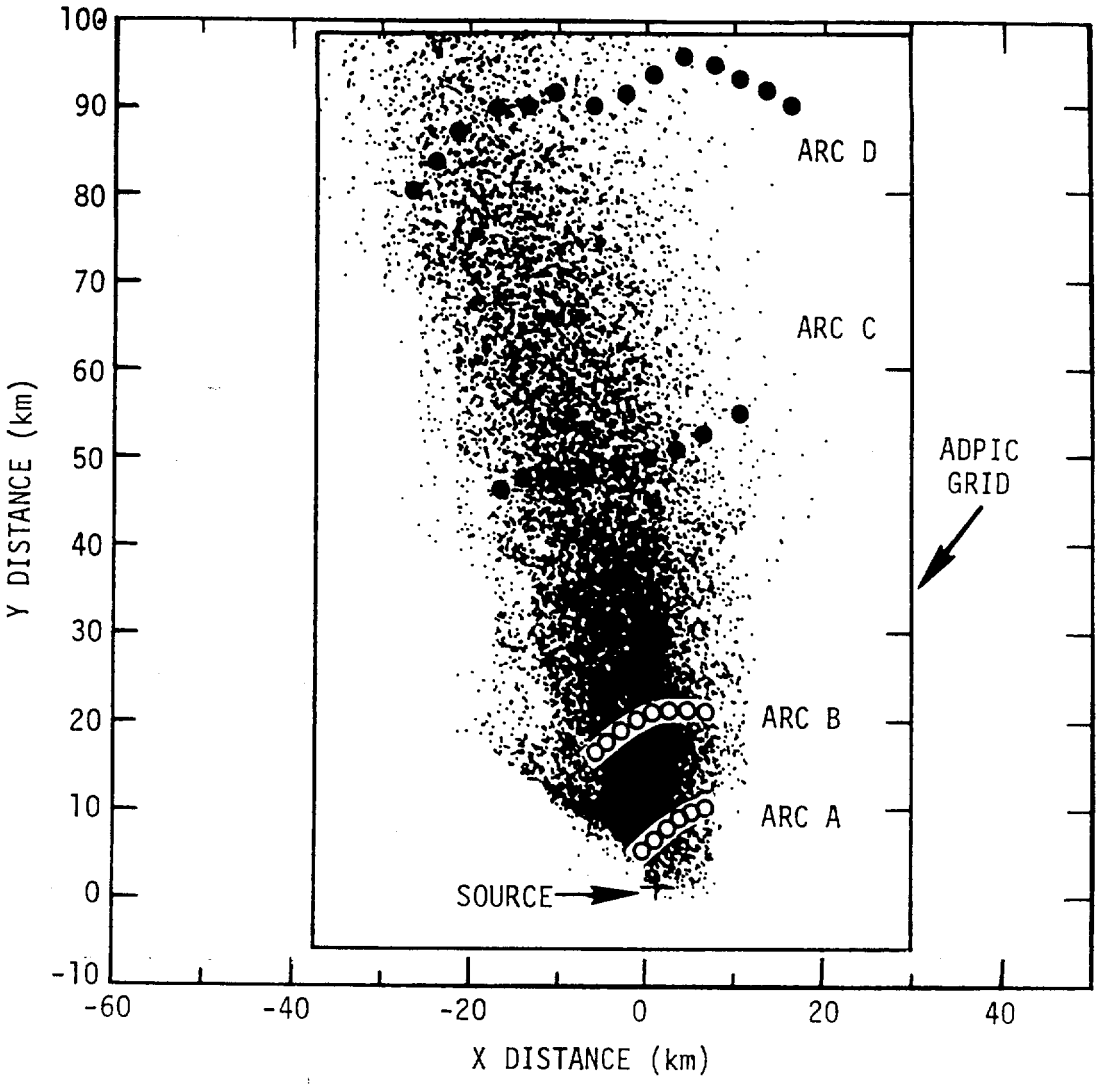
0023862

FIGURE 13. C, K, and P plume activity isopleths from ADPIC for Test 2, 13:00 EDT.

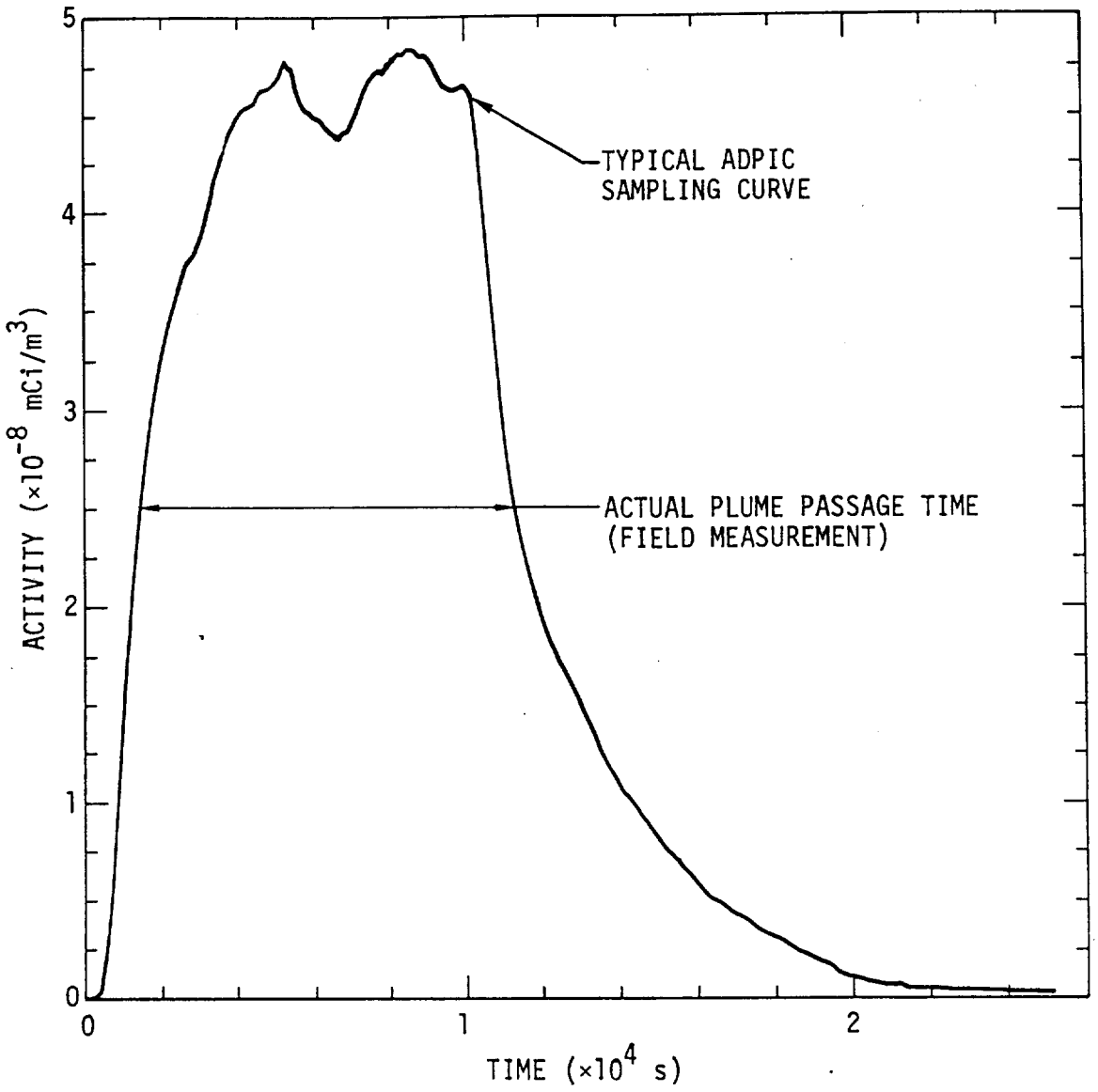
0023863


PLUME
ADPIC GRID SIZE
68.8 X 103.2 km
SOURCE
INTERPOLATED
WINDFIELD
GRID SIZE
103.2 X 129 km

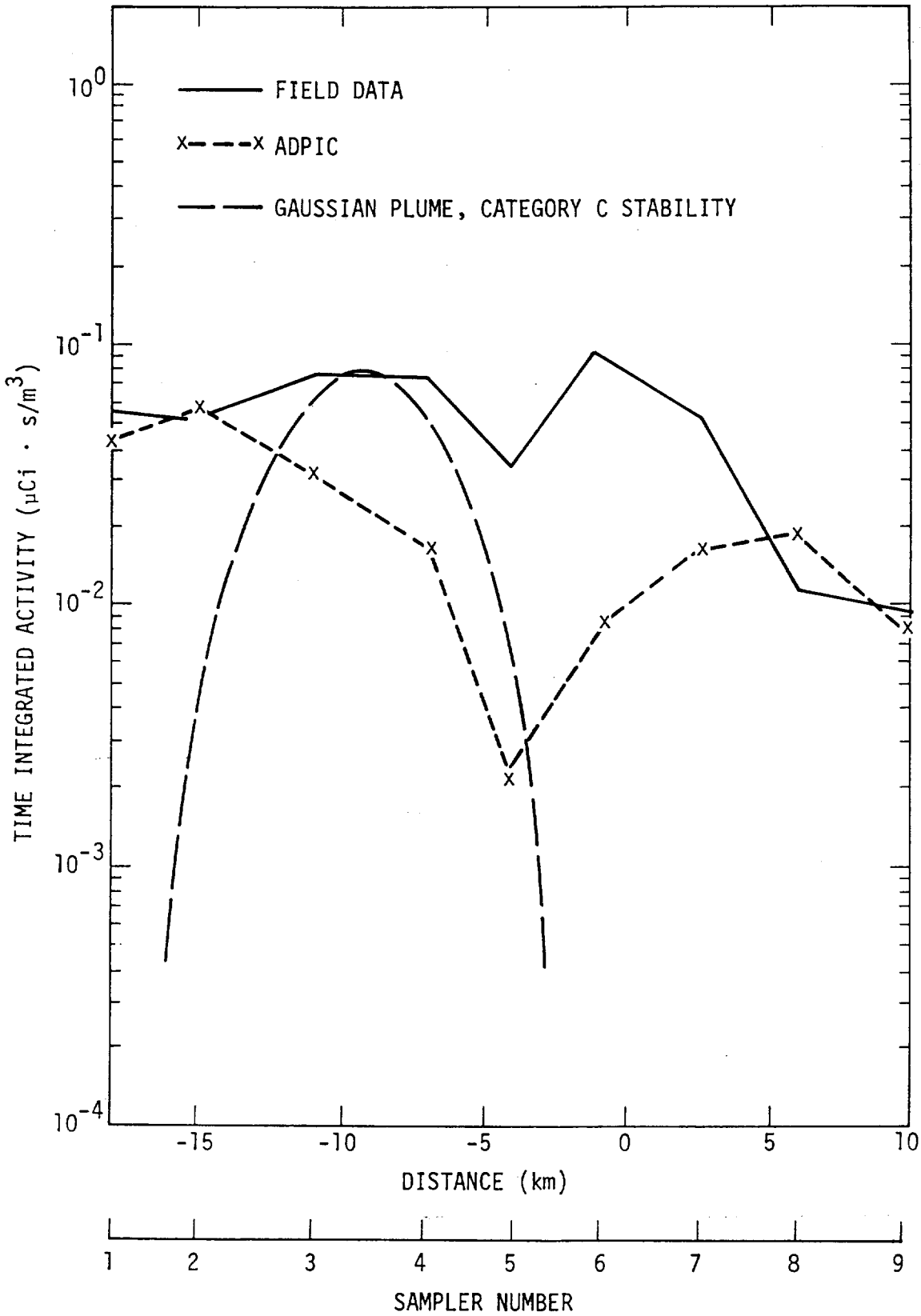
Lange - Fig. 1


100
90
80
70
60
50
40
30
20
10
0
-10
Y DISTANCE (km)
-60
-40
-20
0
20
40
X DISTANCE (km)
ARC D
ARC C
ADPIC
GRID
ARC B
ARC A
SOURCE

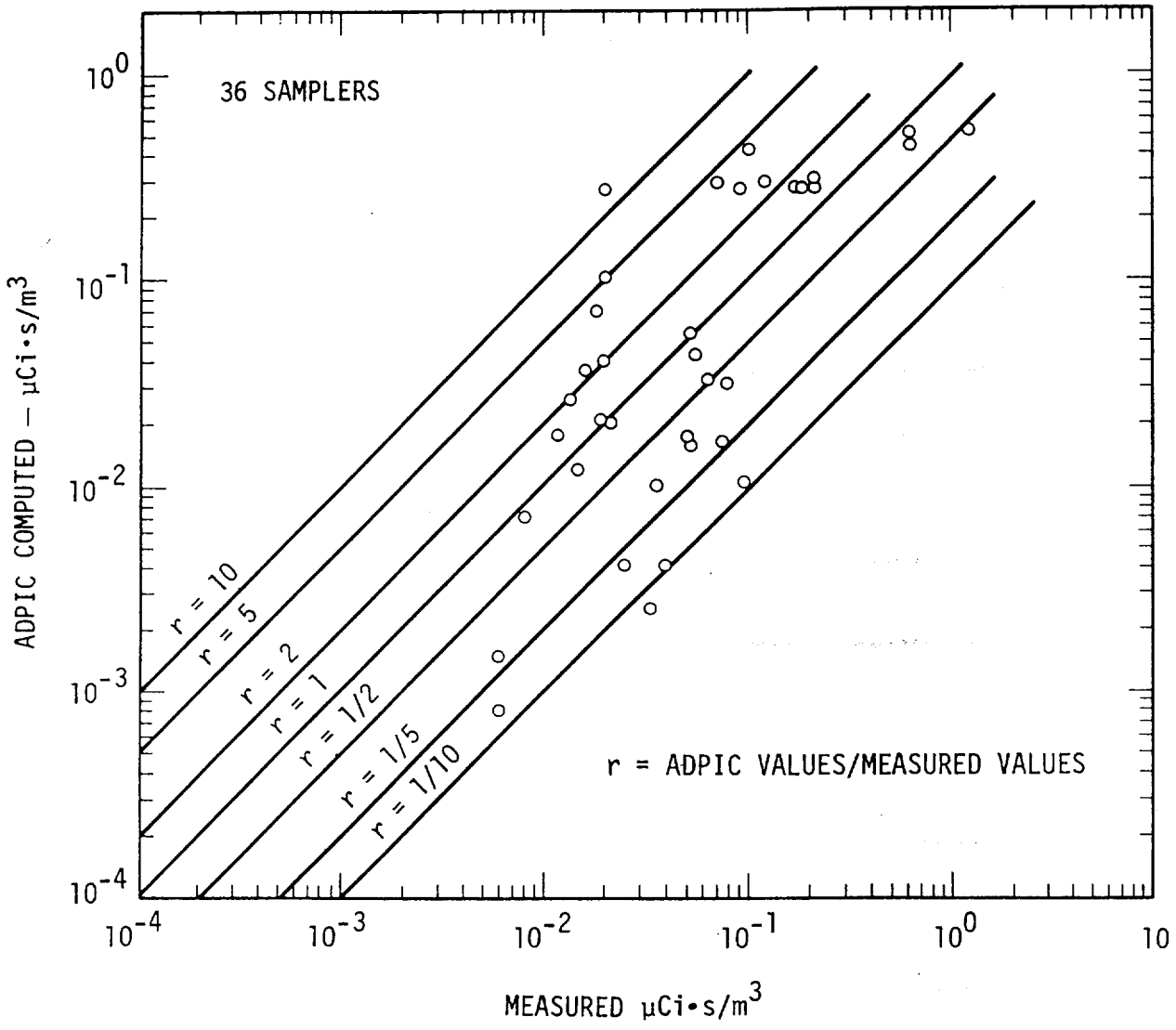
Lange - Fig. 2


5
4
3
2
1
0
ACTIVITY (×10^-8 mCi/m^3)
0
1
2
TIME (×10^4 s)
TYPICAL ADPIC
SAMPLING CURVE
ACTUAL PLUME PASSAGE TIME
(FIELD MEASUREMENT)

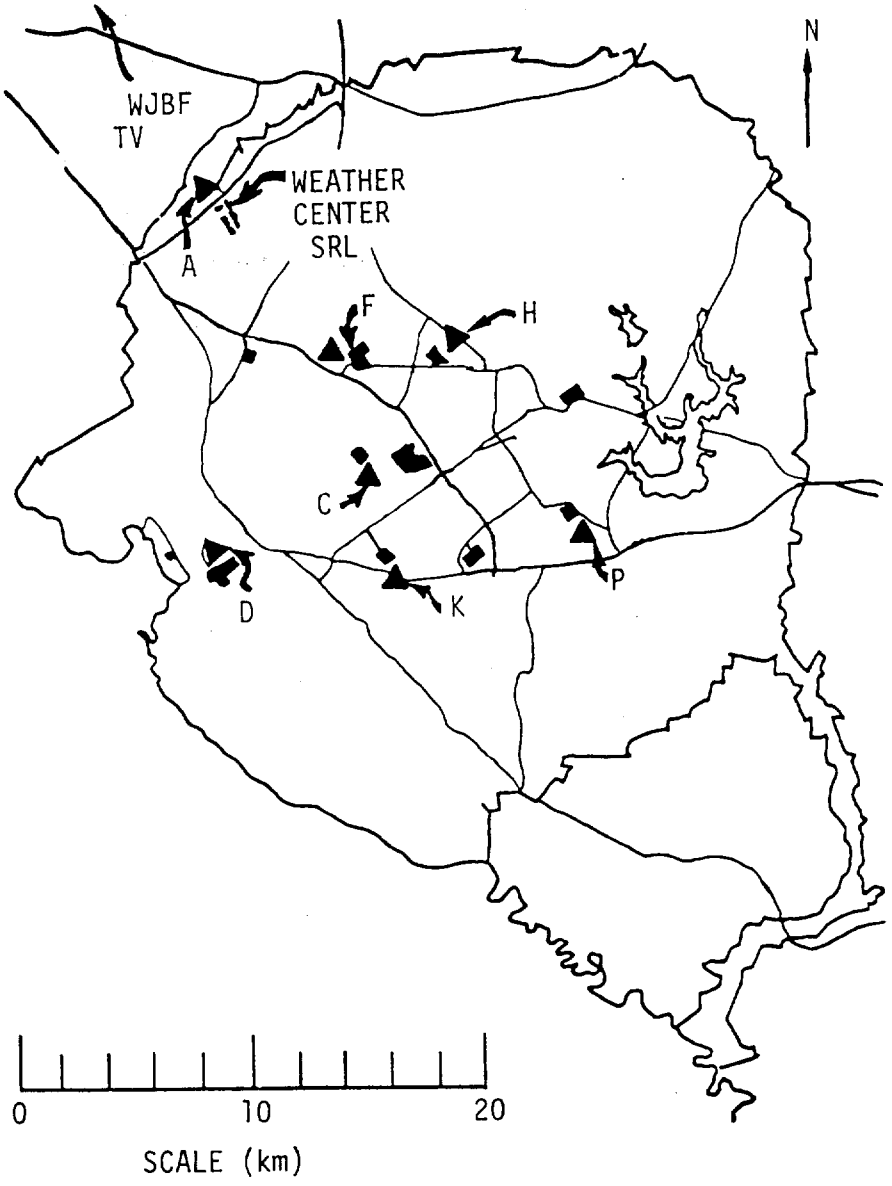
Lange - Fig. 3


FIELD DATA
ADPIC
GAUSSIAN PLUME, CATEGORY C STABILITY
TIME INTEGRATED ACTIVITY (μCi · s/m³)
10⁰
10⁻¹
10⁻²
10⁻³
10⁻⁴
-15
-10
-5
0
5
10
DISTANCE (km)
1
2
3
4
5
6
7
8
9
SAMPLER NUMBER

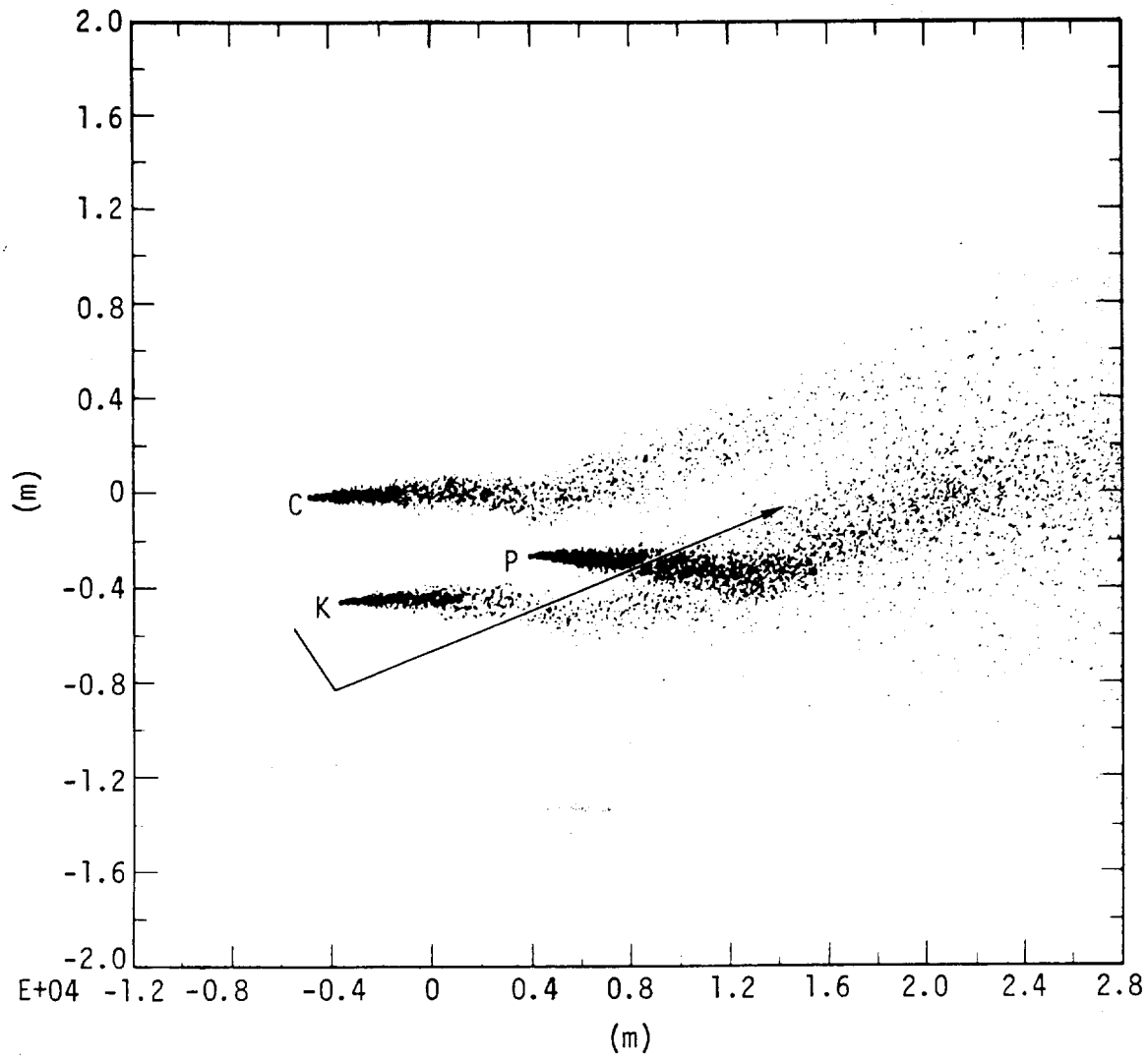
Lange - Fig. 4


36 SAMPLERS
r = 10
r = 5
r = 2
r = 1
r = 1/2
r = 1/5
r = 1/10
r = ADPIC VALUES/MEASURED VALUES
ADPIC COMPUTED — μCi•s/m3
MEASURED μCi•s/m3
10^0
10^-1
10^-2
10^-3
10^-4
10^-4
10^-3
10^-2
10^-1
10^0
10

Lange - Fig. 5

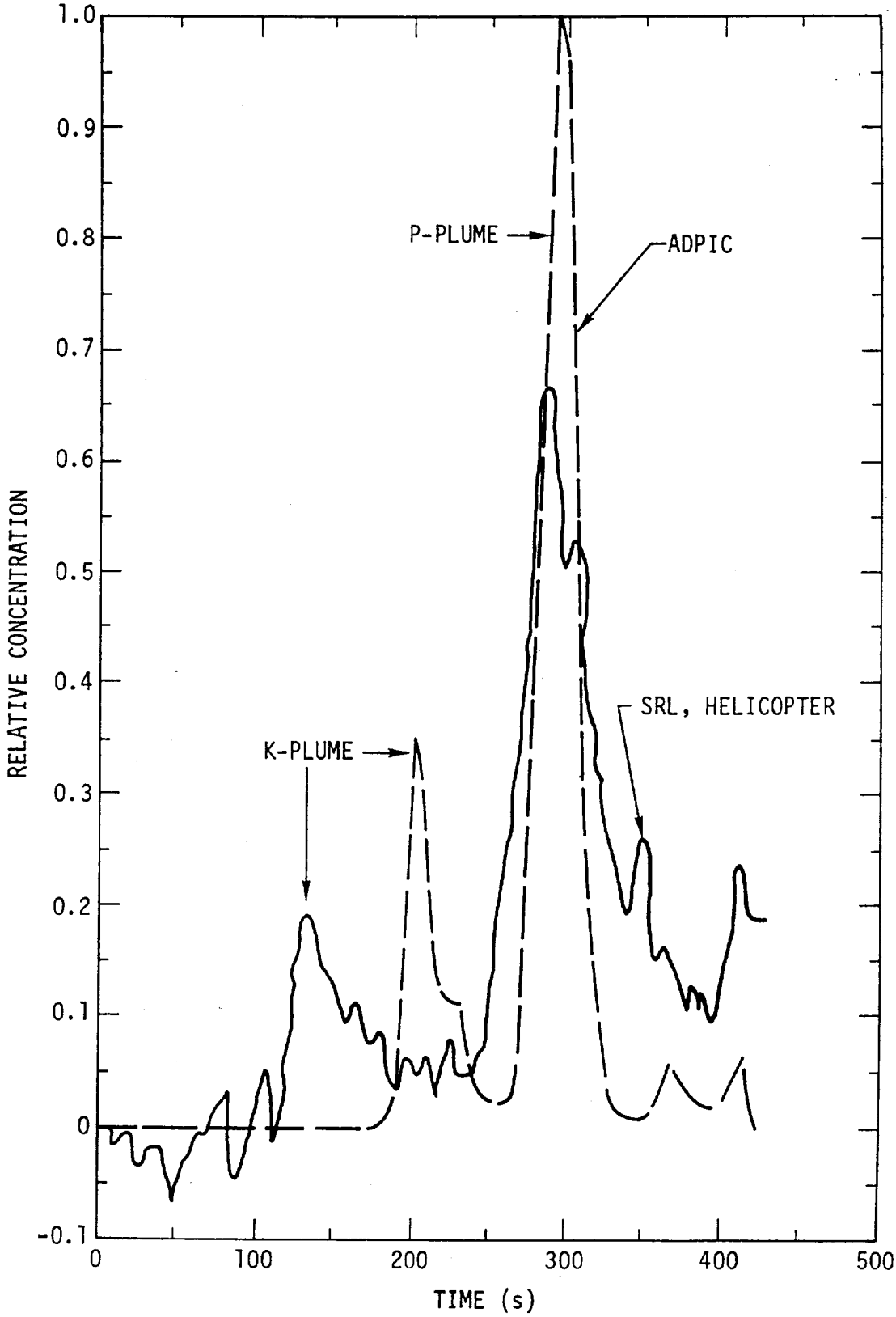


Lange - Fig. 6



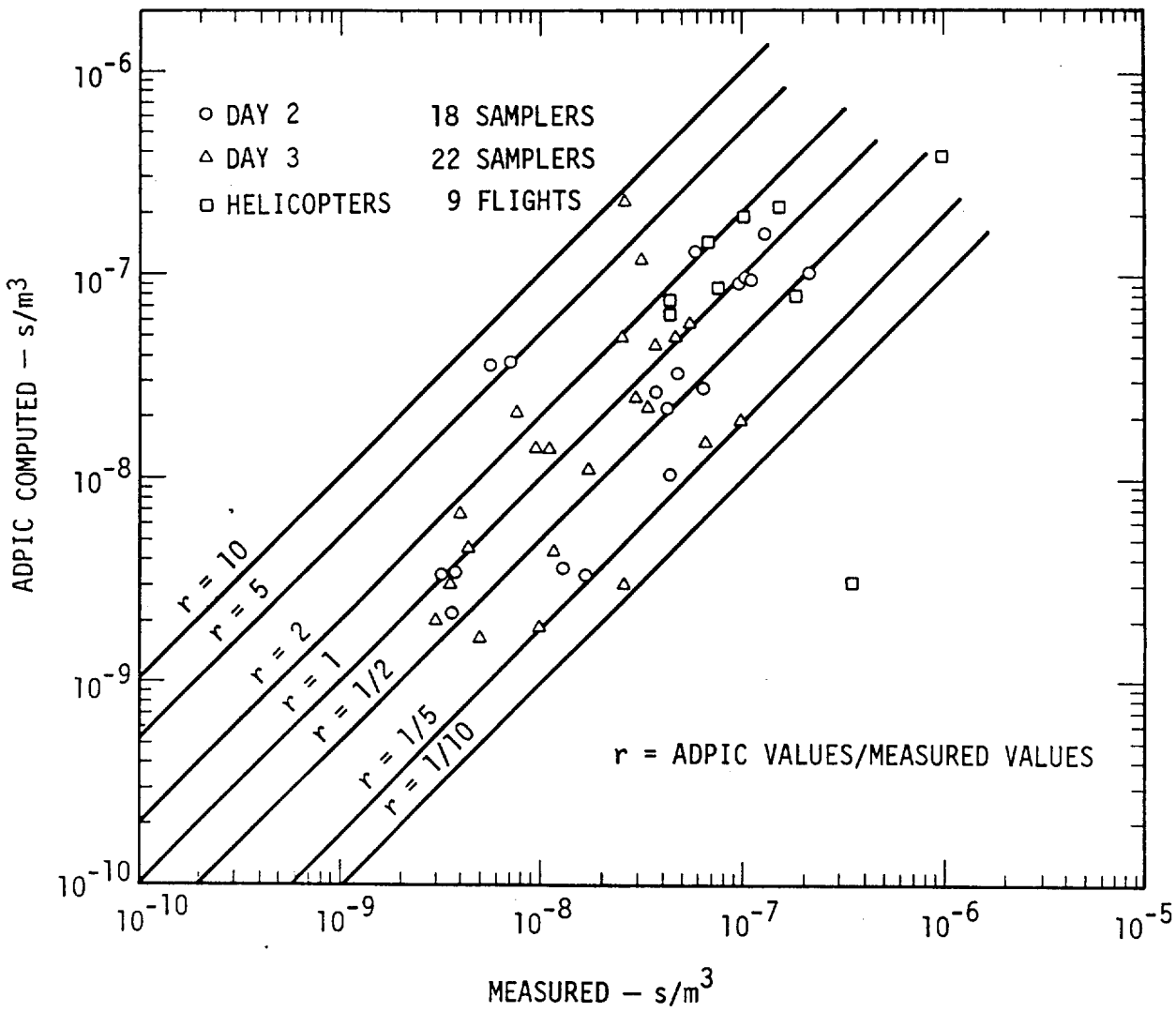
TOTAL x - y PLANES CYCLE95 TIME 1.388E+04 s #838

Lange - Fig. 7



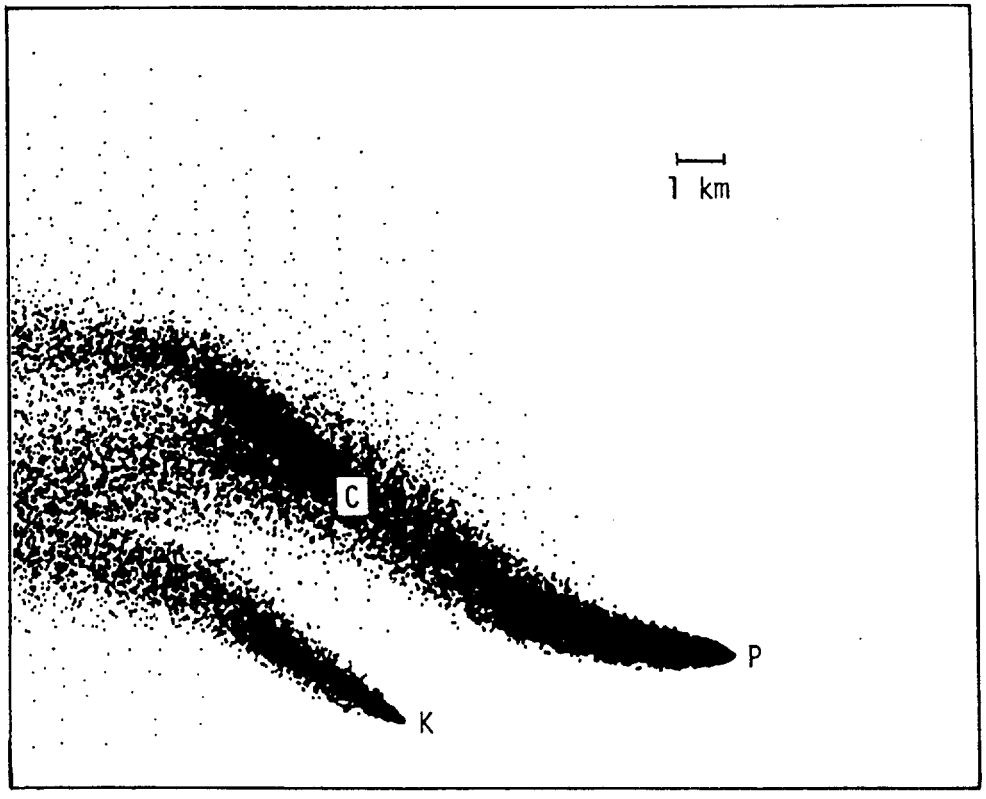
Lange - Fig. 8

0023871



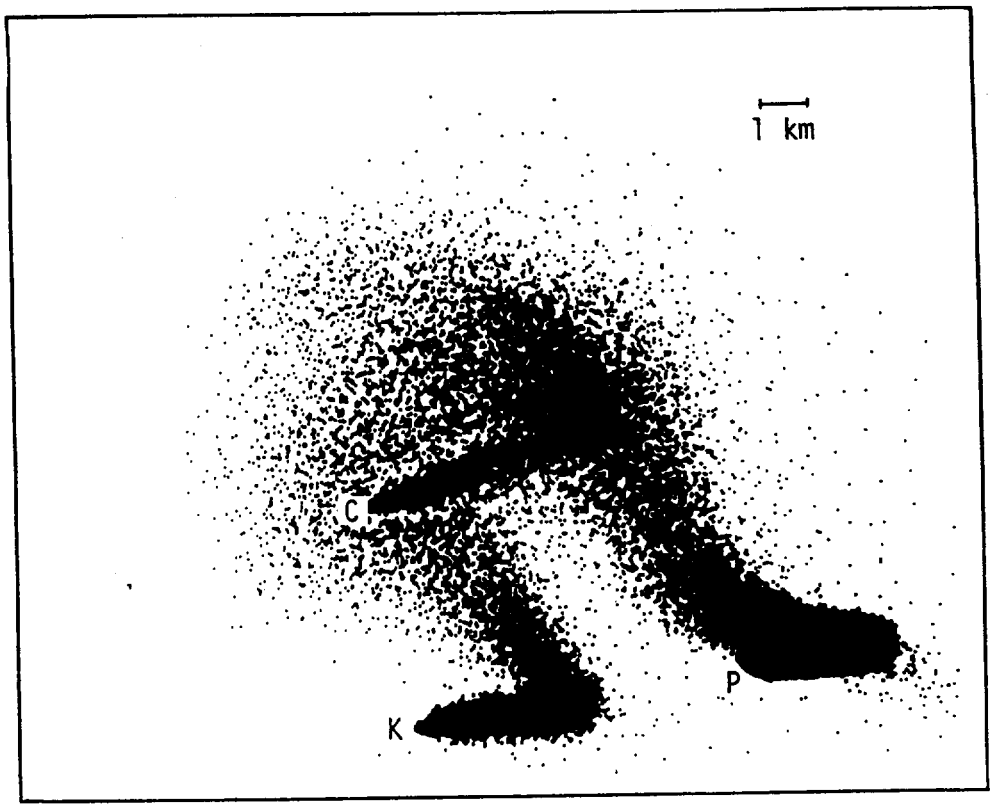
Lange - Fig. 9

0023872



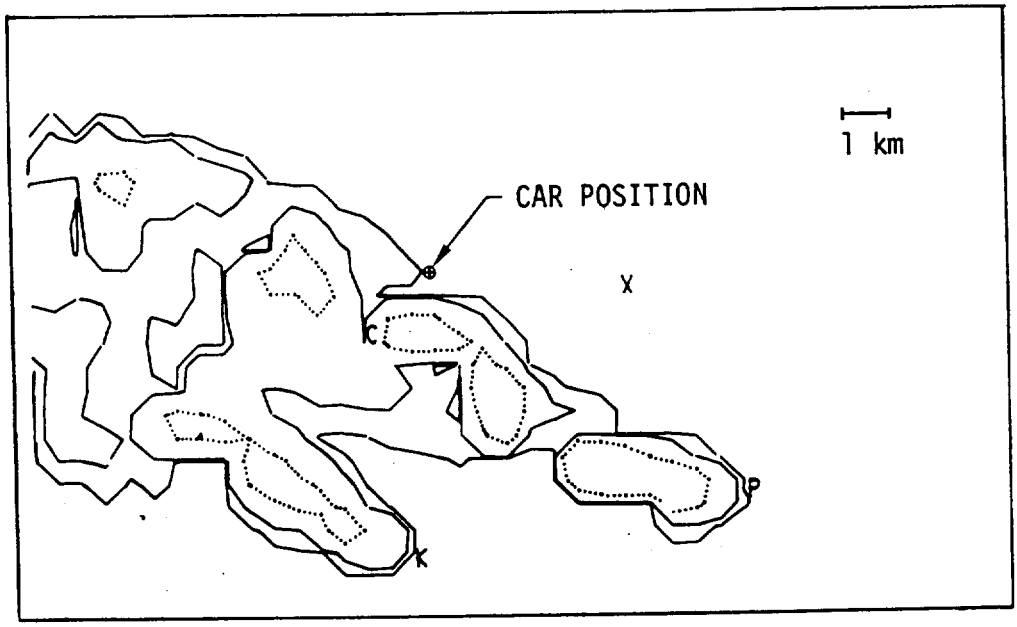
TOTAL x - y PLANES CYCLE230 TIME 12:00 EDT

Lange - Fig. 10



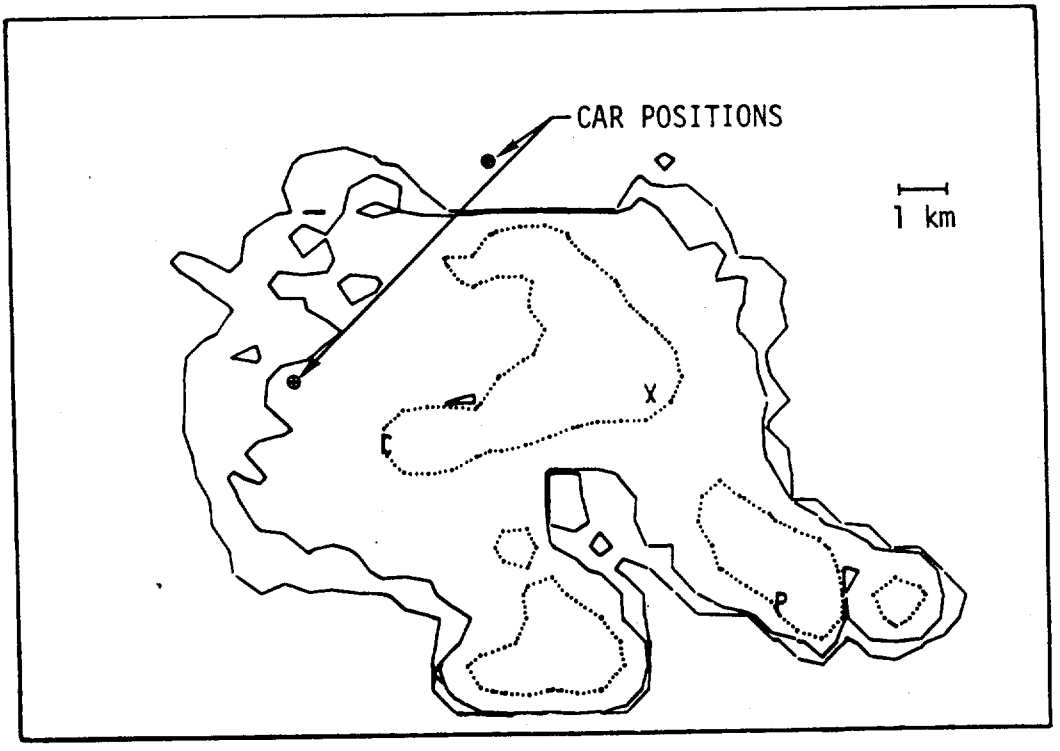
TOTAL x - y PLANES CYCLE258 TIME 13:00 EDT

Lange - Fig. 11



RELATIVE CONCENTRATION AT 2. METERS TIME IS 5.0 HOURS
ISOPLETHS 5×10^{7} 5×10^{-8} 5×10^{-9} s/m^3

Lange - Fig. 12



RELATIVE CONCENTRATION AT 2. METERS TIME IS 6.0 HOURS
ISOPLETHS 5×10^{-7} 5×10^{-8} 5×10^{-9} s/m^3

Lange - Fig. 13

0023876

DISTRIBUTION

Internal

R. Lange	(50 copies)
G-Division	(3 copies)
TID Files	(5 copies)

"Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Energy Research & Development Administration to the exclusion of others that may be suitable."

NOTICE

"This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research & Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights."

0023877

Technical Information Department
LAWRENCE LIVERMORE LABORATORY
University of California | Livermore, California | 94550

PLEASE DO NOT RE-ROUTE
RETURN TO: REPORTS LIBRARY L-53

TO:	L-NO	DUE DATE
R. Hunt	610	5-18-94

174 258
c. 3

CIRCULATION COPY
SUBJECT TO RECALL
IN TWO WEEKS

RECEIVED
LAWRENCE LIVERMORE LABORATORY
DEC 6 1979
TECHNICAL INFORMATION DEPARTMENT

0023878