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Final Report

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LAGRANGIAN MODELING OF TRACER EXPERIMENTS IN THE LOS ANGELES BASIN

Prepared for

Southern California Edison Company Post Office Box 800 2244 Walnut Grove Avenue Rosemead, CA 91770

February 1987

AeroVironment Inc.

825 Myrtle Avenue • Monrovia, California 91016-3424 • USA Telephone 818/357-9983

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Post Office Box 800
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Ву

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February 1987

EXECUTIVE SUMMARY

This report presents the results of the study "Lagrangian Modeling of Tracer Experiments in the Los Angeles Basin" performed by AeroVironment Inc. (AV) for Southern California Edison (SCE). This study involved selecting and analyzing the available tracer data from the Los Angeles Basin, then simulating these tracer experiments using an improved version of the AVACTA II model. The outputs of AVACTA II were then compared with both SF₆ tracer data and the output of ISCST, a simpler regulatory model.

The project was divided into six tasks as discussed below.

- Task 1. We analyzed the available tracer experiments in the Los Angeles Basin. From the available data, we selected three days of the Alamitos experiment (October 17, 25 and 30, 1974), then prepared all the data collected (or available) during these days according to the format requirements of the AVACTA II package.
- o <u>Task 2.</u> We modified and improved the AVACTA II package by adding several controls and options to the program and incorporating the new plume rise algorithm proposed by Turner (1985).
- Task 3. We applied AVACTA II and ISCST to simulate SF₆ dispersion during the three selected days and compared the model's outputs with the ground-level SF₆ measurements available. The models were not successful in simulating the complex hourly variation of the concentration field. AVACTA II did, however, predict the hourly maximum ground-level concentration impact well, while ISCST outputs sometimes largely overestimated the measured values.
- o <u>Task 4.</u> We prepared a new user's manual of AVACTA II that incorporates all the modifications made during this project.

- Task 5. We investigated algorithms and methodologies for developing a "climatological" version of AVACTA II, able to provide a cost-effective simulation of long-term concentration impacts (e.g., annual averages). Several possible approaches were identified and discussed.
- o <u>Task 6.</u> We prepared a comprehensive final report for this project, which includes a full description of all collected data.

In addition to the above tasks, we implemented a personal computer version of AVACTA II that was given to SCE for future applications.

The major conclusion of this study is the evidence of a better performance of dynamic methodologies (such as AVACTA II) versus steady-state assumptions (such as ISCST and most of the EPA "preferred" models). In particular, the similarity between the highest hourly concentration simulated by AVACTA II (with Briggs urban sigmas) and the highest hourly measured concentration is encouraging (115.9 ppb versus 121.0 ppb on October 17, and 165.3 ppb versus 164.0 ppb on October 25), even though this positive behavior is not confirmed on October 30. In comparison with ISCST outputs, the concentration simulated by AVACTA II shows more reasonable fluctuations within an acceptable range. ISCST outputs sometimes largely overestimate the maximum ground level concentration impact, as on October 25. This behavior is certainly a consequence of the steady-state assumption used by ISCST, while AVACTA II allows a dynamic, time-varying treatment of the trajectory of the plume in which the plume is subjected to horizontal meandering instead of remaining steady during each hour of simulation.

ACKNOWLEDGMENTS

We express our gratitude to Southern California Edison (SCE) for sponsoring this modeling study (SCE reference: P.O. C2005903) and acknowledge the technical support provided by Mr. Stan Marsh (SCE Project Manager) and Mr. Vince Mirabella in performing this investigation.

We are grateful to Mr. Joe Griffiths, Ms. Ann Marie Shepard, Ms. Kim Smith, Mr. Gary Arcemont, Mr. Alex Barnett and Mr. John Bongiovanni for their help in data organization, analysis and display. Mr. Bill Moreland has provided a valuable meteorological analysis and meteorological data interpretation.

Finally, we thank Ms. Sandy Reilly for her preparation of this technical report and Ms. Anita Spiess for editorial review.

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1. INTRODUCTION

Southern California Edison (SCE) has sponsored this study, performed by AeroVironment (AV), in order to provide an absolute and relative evaluation of the short-term forecasting performance of AVACTA II, a Gaussian mixed segment-puff model developed by Zannetti et al. (1981, 1986). The absolute evaluation was obtained by comparing AVACTA II output concentrations with SF₆ tracer measurements, while the relative evaluation was made by comparing AVACTA II outputs with those of a standard steady-state Gaussian model (the ISCST model).

The project consisted of six tasks:

- Task 1: Analysis of available tracer data in the Los Angeles Basin and selection of three days for multi-hour simulations. Preparation of the input data (emission, domain, meteorology, options) in the format required by the AVACTA II code.
- Task 2: Modification and improvement of the AVACTA II package.
- Task 3: Running of AVACTA II with input data from the three selected days and absolute/relative statistical evaluation of AVACTA II performance.
- Task 4: Preparation of the new AVACTA II user's manual.
- Task 5: Investigation and discussion of the methodologies required for a possible future implementation of a long-range (climatological) version of AVACTA II.
- Task 6: Report preparation.

The next chapter describes the conclusions of our study, while the following chapters (three through seven) describe the first five tasks above. In Chapter 8 we recommend future research efforts to complement and expand the present study.

To facilitate the reading of this final report, some material (e.g., data, user's manual, etc.) has been presented in the appendices.

2. CONCLUSIONS

We have performed Lagrangian modeling simulation of SF₆ tracer experiments in the Los Angeles basin. Three days, October 17, 25 and 30, 1974 of the SCE Alamitos Generating Station tracer experiment, were selected for these simulations. The simulation outputs of our AVACTA II model, a Lagrangian dynamic segment/puff Gaussian model, were compared with the output of the ISCST model, a standard, steady-state Gaussian model, and with tracer measurements in the region.

Due to the uncertainties in the evaluation of the plume trajectory and to the lack of spatial resolution of the receptors in the region, a quantitative evaluation of the hourly simulation performance of the models was not possible. However, AVACTA II showed an encouraging ability to predict the hourly maximum ground-level impact well, for at least two (October 17 and 25) of the three days of the simulation. On the third day (October 30) both AVACTA II and ISCST underestimated the highest hourly impact (about 30 to 60 percent below the measured value). AVACTA II also predicted ground-level concentrations within a range of values relatively close to the measured data, while ISCST, due to its steady-state assumption, sometimes largely overestimated ground-level impact, as, for example, on October 25, when the highest predicted concentration is about six times the highest measured value.

In conclusion, this study provides further evidence of the necessity of using dynamic methodologies (such as AVACTA II) instead of steady-state methods (such as ISCST and most of the EPA "preferred" models) in order to provide numerical simulations that 1) are a more accurate representation of the physics of dispersion phenomena and 2) are not affected by the overestimation errors sometimes generated by the steady-state assumption.

3. TASK 1 -- ANALYSIS AND SELECTION OF AVAILABLE TRACER DATA, AND PREPARATION OF THE AVACTA II INPUT FILES

We have collected and analyzed the available data from two tracer experiments: Alamitos Generating Station (1974) and Lucerne Valley (1981). Our analyses showed that the Alamitos experiment was the most suitable one for our purposes, since the Lucerne experiment was characterized by light winds and, consequently, by large uncertainties in the wind direction pattern. We, therefore, focused our attention on the Alamitos data. We identified three days suitable for our analyses: October 17, 25 and 30, 1974. The data collected during these days were organized in the format required by the AVACTA II model. This preparation required, among other things:

- The definition of the computational domain and the establishment of a grid reference system.
- 2. The collection of detailed maps covering the Los Angeles Basin region.
- 3. The calculation of terrain elevations in each grid cell using a five-point averaging technique.
- 4. The identification of the UTM coordinates of receptors and meteorological stations.
- 5. The collection of surface meteorological data from 11 stations in the Los Angeles Basin.
- 6. The collection of vertical atmospheric profiles of winds and temperature in the Los Angeles Basin, particularly radiosonde data at El Monte and LAX airports and pibal measurements collected during the tracer experiment program.
- 7. Organization of all the above data in the format (and units) required by the AVACTA II code.

A data report containing all the collected data is presented as Appendix A. The AVACTA II input files are listed as Appendix B.

4. TASK 2 -- MODIFICATION AND IMPROVEMENT OF THE AVACTA II PACKAGE

In this study we used Release 3 of the AVACTA II air pollution package (Zannetti et al., 1986). This version of the code has been successfully evaluated by the EPA and has been proposed as an "alternative" model by the EPA (Dicke, personal communication).

During this study we improved the code by making several modifications to its input files and computational options. We also incorporated into the code the McElroy and Pooler (1968) sigma functions and the Turner (1985) multi-layer plume rise calculation. Both computations can be optionally performed by the user.

The Turner (1985) plume rise method (see the paper enclosed as Appendix C) is a technique for the calculation of plume rise and partial/total penetration through atmospheric layers. It assumes that temperature and wind speed are available from at least two levels above the ground.

We obtained a preliminary version of the Turner (1985) plume rise FORTRAN program from the EPA. We tested it, corrected a few minor inaccuracies in the code and restructured the program into a generalized subroutine inside AVACTA II. The listing of this subroutine is enclosed as Appendix D.

The final AVACTA II program, with all the above improvements, is now referred as Release 3.1 of the computer package.

5. TASK 3 -- ABSOLUTE AND RELATIVE EVALUATION OF AVACTA II

AVACTA II simulations were performed using the meteorological and plume height data collected during the tracer experiments. The two sets of plume sigma functions selected were the Pasquill-Gifford-Turner sigmas and the Briggs urban (i.e., McElroy-Pooler) sigmas. The AVACTA II input files used in these simulations are enclosed as Appendix B (these files refer to the Pasquill-Gifford-Turner sigmas; two records need to be modified to use another set of sigmas; see the AVACTA II User's Guide enclosed as Appendix F, Section 5.1 points 13 and 14).

The analysis of the hourly AVACTA II simulated concentrations against the ground-level SF₆ tracer data produced unsatisfactory results. We analyzed these data and reached the following conclusions:

- 1. The meteorological module (WEST) of AVACTA II seems able to simulate the general wind flow in the region realistically, even though surface layer measurements were used to characterize the transport pattern of the elevated plume at about 300 to 600 m (agl).
- 2. Minor errors in wind direction calculations produce plume trajectories that deviate from the measured ones, with the consequence of simulating hourly plume impacts in the wrong receptors or in areas without receptors.

This situation is not uncommon in air pollution simulation studies. Plume trajectory uncertainties are a major problem in most evaluation studies and methods have been proposed to deal with this problem as discussed below.

The most common way of treating wind direction uncertainties in model validation studies is to force the simulated plume along the <u>measured</u> plume trajectory (i.e., see Zannetti et al., 1982). This methodology allows the validation of plume dispersion parameters by removing the uncertainty related to the actual location of the plume. Especially for regulatory applications, where what counts is the maximum plume impact and not necessarily its location, this method is quite

acceptable. In this present study, however, this approach cannot be used due to the limited spatial resolution of the SF₆ measurement locations. In other words, we do not have detailed ground-level measurements of plume crosswind concentration distribution (i.e., plume transections) to allow a clear determination of the center and the horizontal size of the plume. This determination would require (Ludwig 1977; Zannetti, 1981) the condition

$$\Delta d \leq \sigma_y$$

to be met, where Δd is the horizontal separation between contiguous receptors and σ_y is the plume horizontal sigma (i.e., the standard deviation of the plume crosswind horizontal concentration distribution). This condition is clearly not met by our present data, since Δd is typically around 10 km and σ_y is always below this value.

A second way of treating this problem is to increase the averaging time, for example by analyzing eight-hour average concentrations instead of hourly ones. This averaging process works well when wind direction errors are random, since it can take advantage of error cancellation effects. But when wind direction errors are systematic (e.g., a systematic difference of about ten degrees between measured and simulated plume trajectories) this averaging process does not substantially increase the performance of the model.

A third way of dealing with this problem is to focus on the highest concentration values (both measured and computed) independently of their location and time (i.e., "uncoupled" comparison). This method (Fox, 1981, and Fox, 1984) has become very common in the evaluation of the "practical" performance of air pollution models for typical regulatory applications.

The period of eight hours was chosen to represent the average conditions throughout the entire daily tracer experiment.

Based on the above considerations, we made some efforts to improve our understanding of the actual performance of AVACTA II, at least on a qualitative basis. Tables 5-1, 5-2 and 5-3 present a summary of eight-hour average concentrations and maximum hourly concentrations for the three days under examination. In addition to the two AVACTA II simulations (for Pasquill-Gifford-Turner and Briggs urban sigma) and the measured data, the tables show the simulation results obtained using the ISCST model in the standard way for regulatory applications. These latter data are presented in order to evaluate both the <u>absolute</u> performance of AVACTA II (i.e., against tracer data) and the <u>relative</u> one (i.e., against another model, ISCST, which is a "preferred" EPA model for regulatory applications).

The analysis of Tables 5-1 through 5-3 does not indicate a clear, identifiable pattern in the data. However, the similarity between the highest hourly concentration simulated by AVACTA II (with Briggs urban sigmas) and the highest hourly measured concentration is certainly encouraging (115.9 ppb versus 121.0 ppb on October 17, and 165.3 ppb versus 164.0 ppb on October 25), even though this positive behavior is not confirmed on October 25. In comparison with ISCST outputs, the concentration simulated by AVACTA II shows more reasonable fluctuations. In fact, ISCST outputs sometimes largely overestimate the maximum ground level concentration impact, as on October 30. This behavior is certainly a consequence of the steady-state assumption used by ISCST, while AVACTA II allows a dynamic, time-varying treatment of the trajectory of the plume in which the plume is subjected to horizontal meandering instead of remaining steady during each hour of simulation.

As noted before, the spatial resolution of the receptors is insufficient to characterize plume trajectory and growth well. Nevertheless, it is certainly worthwhile to look at the entire concentration field generated by AVACTA II. Figures 5-1 through 5-6 show the isopleths of the eight-hour average ground-level SF₆ concentrations simulated by AVACTA II (for both Pasquill-Gifford-Turner

The period of eight hours was chosen to represent the average conditions throughout the entire daily tracer experiment.

TABLE 5-1. Computed and measured ${\rm SF}_6$ concentrations on October 17 (ppb).

Doctor No	Averag	Average 8 Hours (entire	re experiment)	nt)		Hour	Hourly Maximum	
(as in Fig. 5-1)	AV-PG ⁽⁰⁾	AV-BU ^(oo)	ISC ^(*)	Measured ⁽⁺⁾	AV-PG	AV-BU	ISC ^(*)	Measured ⁽⁺⁾
1	0.0	0.0	0.0	3.0	0.0	0.0	0.0	5.1
2	0.0	0.0	0.0	15.7	0.1	0.0	0.0	85.5
3	0.0	0.0	0.0	1.5	0.0	0.0	0.0	4.1
4	1.0	0.0	0.0	30.5	8.9	7. 0	0.0	121.0
2	7.1	14.5	29.9	17.0	56.4	115.9	87.6	4.89
9	0.0	0.0	0.0	9.5	0.0	0.0	0.0	22.1
7	0.0	0.0	0.0	2.7	0.0	0.0	0.0	6.6
∞	0.0	0.0	1	29.2	0.0	0.0	ı	107.0
6	0.0	0.0	1	0.9	0.0	0.0	1	25.0
10	0.0	0.0	0.0	6.7	0.0	0.0	0.0	14.9
11	0.0	0.0	•	6.3	0.0	0.0	ı	7.9
12	0.2	0.0	1	ı	1.2	0.0	ı	
13	0.1	0.0	ı	•	0.7	0.0	1	•
14	0.0	0.0	ı	•	0.0	0.0	1	•
15	19.7	15.7	0.0	t	110.0	71.1	0.0	1
16	0.2	0.0	ı	3.5	1.3	0.0	ı	5.5
17	1.9	1.6	1	33.6	14.8	12.6	1	61.0
18	0.0	0.0	0.0	10.7	0.3	0.0	0.0	28.7
19	0.0	0.0	ţ	2.5	0.0	0.0	ı	6.2
20	0.0	0.0		•	0.0	0.0	•	ı
21	0.0	0.0	1	7.3	0.0	0.0	•	19.0
22	0.0	0.0	t	8.9	0.0	0.0	ı	12.0
Highest	19.7	15.7	29.9	33.6	110.0	115.9	87.6	121.0

Missing values indicate that the receptors are located above the height of the release and, therefore, cannot be simulated by ISC. *

⁽⁺⁾ Missing values indicate that data were not collected.

⁽o) AVACTA II with Pasquill-Gifford sigmas

⁽⁰⁰⁾ AVACTA II with Briggs urban sigmas

TABLE 5-2. Computed and measured ${\rm SF}_6$ concentrations on October 25 (ppb).

	Average	Average 8 Hours (entire	re experiment)	nt)		Hourl	Hourly Maximum	
Receptor No. (as in Fig. 5-1)	AV-PG(0)	AV-BU ⁽⁰⁰⁾	ISC ^(*)	Measured ⁽⁺⁾	AV-PG	AV-BU	ISC(*)	Measured ⁽⁺⁾
_	0	0.0	0.0	0.7	0.0	0.0	0.0	1.4
	36.6	43.9	0.0	52.2	126.4	165.3	0.0	127.0
1 ~	0.0	0.0	2.9	2.2	0.0	0.8	22.9	13.0
t	37.3	34.0	4.46	56.7	105.8	95.6	625.1	164.0
- 50	0.1	0.0	7.6	1.4	0.9	10.4	75.8	9.4
9	0.1	0.0	0.0	1.4	0.3	0.1	0.0	•
· _	0.0	0.0	157.8	5.9	0.0	0.0	1012.1	24.5
. ∞	4.7	2.5	ı	28.4	23.8	18.2	ı	53.2
6	2.0	0.0	ı	6.1	14.4	0.0	1	28.0
01	0.0	0.0	0.0	0.1	0.0	0.0	0.0	7.2
: =	0.0	0.0	ı	0.7	0.0	0.0	•	2.2
12	0.5	0.0	ı	•	3.0	0.0	i	1
13	31.4	9*9	ı	ı	81.9	29.3	ı	1
14	0.0	0.0	ı	ı	0.0	0.0	ı	ı
15	10.9	17.4	67.1	ı	37.5	61.2	182.4	1
16	1.2	0.0	1	1.7	9.6	0.0	ı	6. 1
17	19.9	18.4	1	20.9	93.5	6.79	ı	6.44
18	4.5	0.1	0.0	•	16.2	0.2	0.27	1
19	0.0	0.0	1	0.3	0.0	0.0	ı	2.6
20	0.0	0.0	ı	ı	0.0	0.0	1	ı
21	0.0	0.0	ı	3.9	0.0	0.0	ı	13.0
22	0.0	0.0	ı	2.2	0.0	0.0	1	6.9
Highest	37.3	43.9	157.8	56.7	126.4	165.3	1012.1	164.0

Missing values indicate that the receptors are located above the height of the release and, therefore, cannot be simulated by ISC. *

(+) Missing values indicate that data were not collected.

(o) AVACTA II with Pasquill-Gifford sigmas

(00) AVACTA II with Briggs urban sigmas

TABLE 5-3. Computed and measured SF $_{6}$ concentrations on October 30 (ppb).

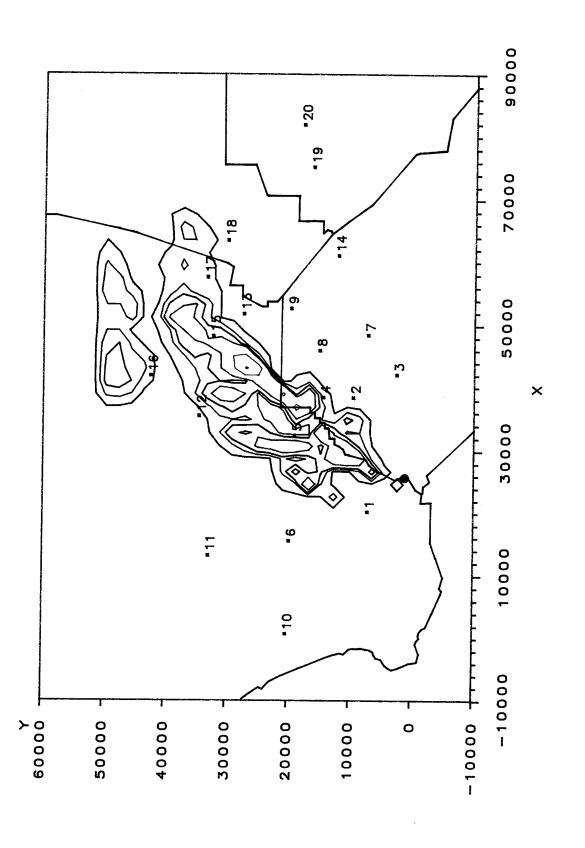
Recentor No.	Averag	Average 8 Hours (entire	re experiment)	nt)		Hour	Hourly Maximum	
(as in Fig. 5-1)	AV-PG ⁽⁰⁾	AV-BU ^(oo)	ISC ^(*)	Measured ⁽⁺⁾	AV-PG	AV-BU	ISC ^(*)	Measured ⁽⁺⁾
1	0.0	0.0	0.0	6 0	0 0			
2	33.9	7 4	30 6	0 (2)	0 0	· ;	0.0	4.1
	, ,	• 6	9.0	6.79	182.2	31.8	238.3	314.0
٦ -	0.0	o ;	0.0	0.0	0.0	0.0	0.0	0.0
+ 1	33.6	31.9	13.7	34.3	136.0	170.8	7 8 9	7.0
٠ <u>٠</u>	4.9	1.3	0.0	3.1	39.2	8.6	, ,	0.01
9	0.0	0.0	0.0	9.0	0.0			7.0
7	0.0	0.0	0.3	0.0		• •		o•7
∞	17.4	2.0	\ •) : :	9 0	o (9.7	I.I
σ	7 0	9 6	ı	74.0	11/.8	15.2	•	67.4
\ <u>-</u>	۲۰۰	0.0	1	0.0	43.9	0.1	,	0.0
o :	0.0	0.0	0.0	3.9	0.0	0.0	0 0	2 6
:	0.0	0.0	•	2.0	0.0	0.0) • •	7 2
12	4.5	4.8	t	3.4	27.5	37.3	ı	· · · · ·
13	38.3	27.4	1		140.7	117.0	I	7.07
14	0.0	0.0	ı	5.0		7. (ı	1 5
15	5.0	2 2	78 1	, ,	•	2 6	1	14.8
<u> </u>) -		1.02	C•7	8.67	32.7	93.7	8.6
12	1.00	/•/		1.9	10.9	77.4		9.4
7 -	1.40	7.47	1	8.9	212.2	92.9	•	15.7
× :	8·9	0.5	8. 8.		50.2	3.7	43.3	
9	0.0	0.0	1	0.0	0.0	0.0	\ \ \ !	c : c
70	0.0	0.0	ı	•	0.0		ı	0.00
21	0.0	0.0	,				ı	1 1
22	0	c		4 (•	0.0	1	6.5
1	•	•	ı	5. 0	0.0	0.0	1	3.6
Highest	39.7	31.9	30.6	62.9	212.2	170.8	238.3	314.0

Missing values indicate that the receptors are located above the height of the release and, therefore, cannot be simulated by ISC. *

(+) Missing values indicate that data were not collected.

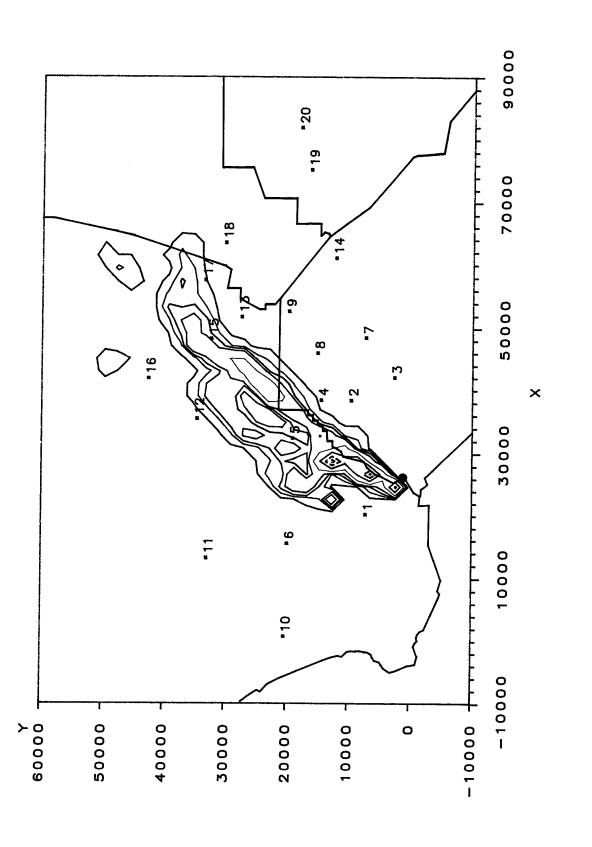
(o) AVACTA II with Pasquill-Gifford sigmas

(00) AVACTA II with Briggs urban sigmas



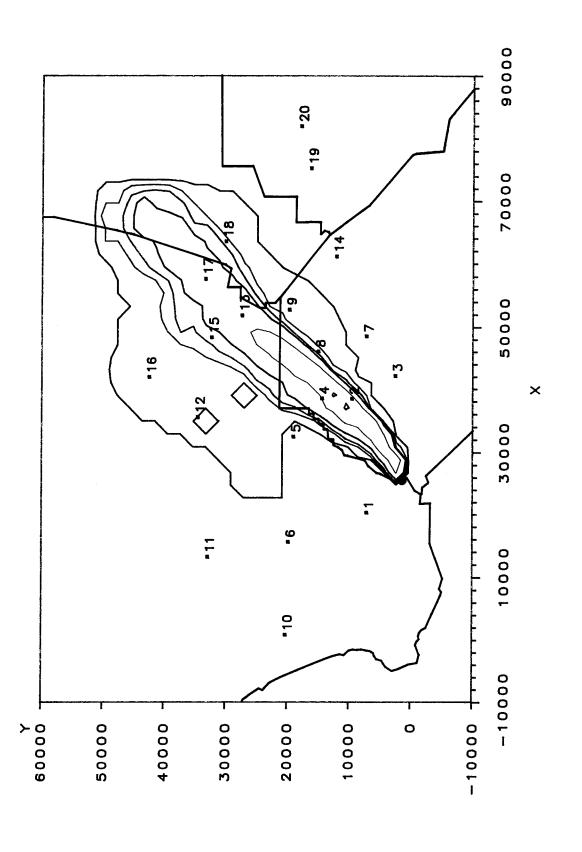
2 0 0 0 0 0 3 3 3 3 3 3 15 CONC

Isopleths of the simulated ground-level SF6 concentration field. The numbers indicate the location of the SF6 monitoring stations. Simulation of October 17, 1984, eight-hour averages, Pasquill-Gifford sigmas. The stack location is depicted by a dot (**). The maximum concentration is 67 ppb at (43000, 27000). FIGURE 5-1.



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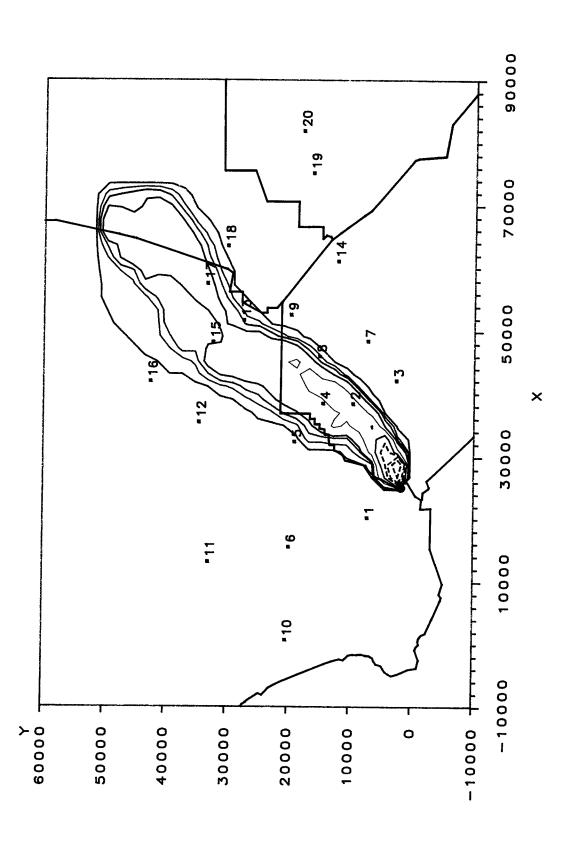
Isopleths of the simulated ground-level SF concentration field. The numbers indicate the location of the SF monitoring stations. Simulation of October 17, 1984, eight-hour averages, Briggs urban sigmas. The stack location is depicted by a dot (**). The maximum concentration is 144 ppb at (29000, 12000). FIGURE 5-2.



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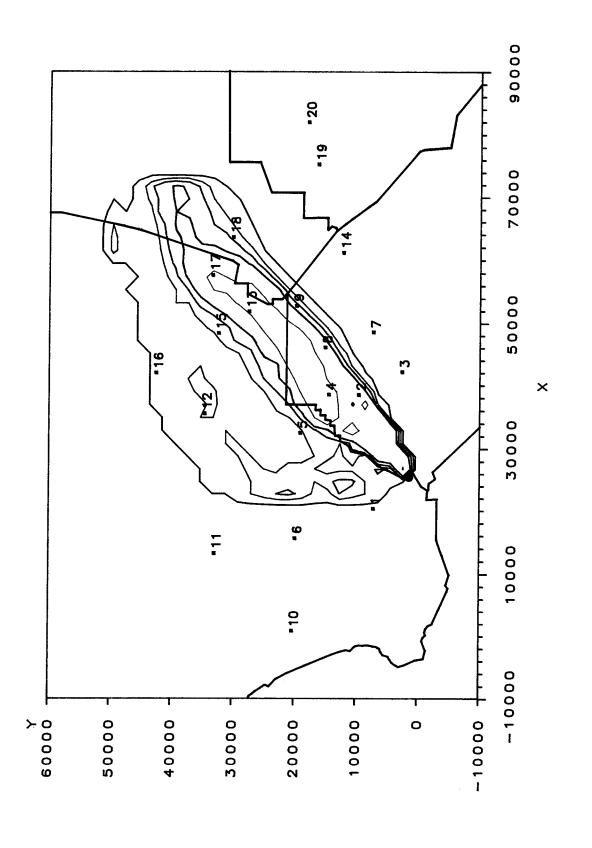
Isopleths of the simulated ground-level SF₆ concentration field. The numbers indicate the location of the SF₆ monitoring stations. Simulation of October 25, 1984, eight-hour averages, Pasquill-Gifford sigmas. The stack location is depicted by a dot (①). The maximum concentration is 69 ppb at (37000, 11000).

FIGURE 5-3.



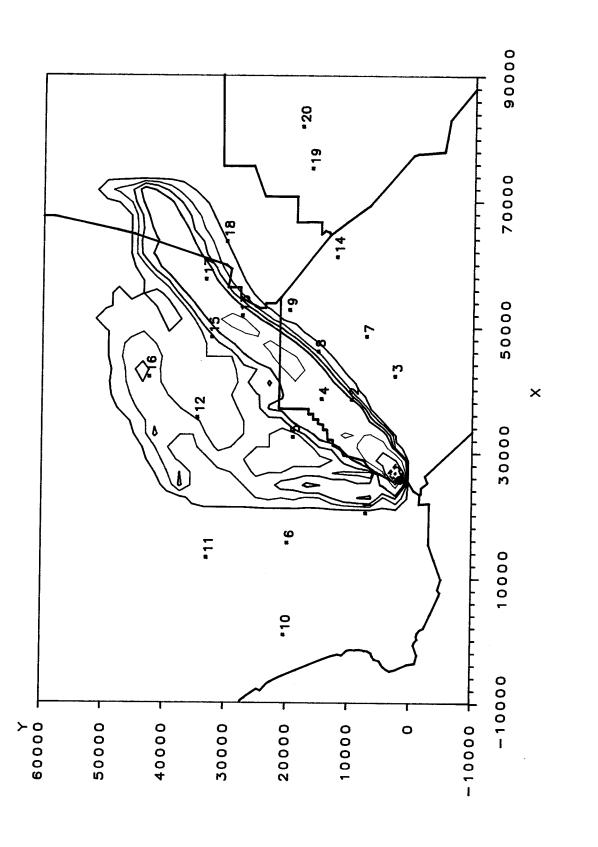
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		!
CONC		

Isopleths of the simulated ground-level SF concentration field. The numbers indicate the location of the SF monitoring stations. Simulation of October 25, 1984, eight-hour averages, Briggs urban sigmas. The stack location is depicted by a dot (**). The maximum concentration is 285 ppb at (29000, 3000). FIGURE 5-4.



6 5 0 0 0 0 3 3 3 5 0 CONC

Isopleths of the simulated ground-level SF₆ concentration field. The numbers indicate the location of the SF₆ monitoring stations. Simulation of October 30, 1984, eight-hour averages, Pasquill-Gifford sigmas. The stack location is depicted by a dot (•). The maximum concentration is 63 ppb at (46000, 20000). FIGURE 5-5.



6 6 2 0 0 0 3 3 3 3 3 15 CONC

Isopleths of the simulated ground-level SF concentration field. The numbers indicate the location of the SF monitoring stations. Simulation of October 30, 1984, eight-hour averages, Briggs urban sigmas. The stack location is depicted by a dot (**). The maximum concentration is 212 ppb at (27000, 2000).

FIGURE 5-6.

5-12

and Briggs urban sigmas). These isopleths illustrate the complexity of the simulated concentration field. Clearly, small errors in wind direction of just a few degrees may carry the centerline of the plume away from the actual area of impact, thus making difficult or impossible a quantitative model evaluation effort.

A satisfactorily quantitative comparison of simulated and measured concentration is clearly difficult, but important quantitative considerations can be derived from the eight-hour average simulations depicted in Figures 5-1 through 5-6, as discussed below for each simulation day.

o October 17 (Figures 5-1 and 5-2)

The maximum eight-hour average concentrations simulated by AVACTA II are 67 ppb (PG sigmas) and 144 ppb (BU sigmas). Both impacts are found at locations quite distant from the receptor points, and, therefore, cannot be compared with actual measurements. The maximum values simulated by AVACTA II at the receptor points are 20 ppb at receptor 15 (PG sigmas) and 16 ppb at receptor 15 (BU sigmas). The maximum measured concentration is 34 ppb at receptor 17, which is relatively close to receptor 15. The ISCST model does not show any impact in the area around receptors 15 and 17; its maximum impact is 30 ppb at receptor 5.

o October 25 (Figures 5-3 and 5-4)

The maximum eight-hour average concentrations simulated by AVACTA II are 69 ppb between receptors 2 and 4 (PG sigmas) and 285 ppb (BU sigmas) very close to the source, where no receptors were located. The maximum values simulated by AVACTA II at the receptor points are 37 ppb at receptor 4 (PG sigmas) and 44 ppb at receptor 2 (BU sigmas). The maximum measured concentration is 57 ppb at receptor 4, while 52 ppb are measured at receptor 2. The ISCST model shows no impact at receptor 2 (0 ppb), a large impact at receptor 4 (94 ppb) and a maximum impact at receptor 7 (158 ppb) where very low concentration is either measured (6 ppb) or simulated by AVACTA II (0 ppb).

o October 30 (Figures 5-5 and 5-6)

The maximum eight-hour average concentrations simulated by AVACTA II are 63 ppb (PG sigmas) in the region near receptors 2, 4, 13 and 17, and 212 ppb (BU sigmas) very close to the source where no receptors are located. The maximum values simulated by AVACTA II at the receptor points are 40 ppb at receptor 17 (PG sigmas; also 34 ppb at receptors 2 and 4, and 38 ppb at receptor 13), and 32 ppb at receptor 4 (BU sigmas; also 27 ppb at receptor 13 and 24 ppb at receptor 17). The maximum measured concentration is 68 ppb at receptor 2. Some impact (34 ppb) is also measured at receptor 4, while much lower impacts are measured elsewhere (measurements, however, were not available at receptor 13). The ISCST model shows a maximum impact (31 ppb) at receptor 2, but a much lower impact (14 ppb) at receptor 4.

From the above discussion we conclude that AVACTA II shows encouraging qualitative and quantitative simulation features that represent an improvement with respect to steady-state Gaussian models, such as ISCST.

We have analyzed the general problem of comparing model outputs with measurements and derived observations and comments that apply to this study. We enclose a draft copy of a report summarizing our views on this subject as Appendix G.

6. TASK 4 -- PREPARATION OF THE NEW AVACTA II USER'S MANUAL

Chapter 4 described the improvements and modifications of the AVACTA ll program performed during this study. Consequently, a new version of the AVACTA ll User's Guide (Release 3.1) was prepared and is enclosed as Appendix F. It contains a paper, recently published on <u>Atmospheric Environment</u>, that fully describes the numerical methods and assumptions of AVACTA ll.

7. TASK 5 -- FUTURE IMPLEMENTATION OF THE LONG-RANGE (CLIMATOLOGICAL) VERSION OF AVACTA II

AVACTA Il is a dynamic model, i.e., a model in which the concentrations predicted at a certain time step are dependent upon the concentration field simulated during the previous time step. Therefore, a "climatological" version of AVACTA Il cannot be defined in a straightforward manner, as in the case of steady-state models. Several computational techniques, however, can be used to allow AVACTA Il to simulate, in a cost-effective manner, long-term concentration averages, without going through expensive hour-by-hour simulations. We expect, in the near future, to implement a "climatological" version of the AVACTA Il code, based on the ideas illustrated below.

7.1 Case 1 - Single Meteorological Station

When only one meteorological station is available in the region, during the period T under investigation, the measured joint frequencies of hourly occurrence f (i, j, k) of the i-th wind speed class, the j-th wind direction sector and the k-th stability class can be used in the following algorithm

$$\bar{c}(r, s) = \frac{\sum_{i, j, k}^{} f(i, j, k) c_{ijk}(r, s)}{\sum_{i, j, k}^{} f(i, j, k)}$$
 (7.1)

where \bar{c} (r, s) is the long-term average concentration in the receptor r due to the source s during the period T, and c_{ijk} (r, s) is the concentration due to the source s simulated by AVACTA II at the receptor r, for the i-th wind speed class, the j-th wind direction and the k-th stability class.

Equation (7.1) is equal to the standard Gaussian climatological model; however, the simulation of c_{ijk} (r, s) by AVACTA II requires:

- 1. Multi-hour simulation under stationary meteorological conditions until a steady-state concentration field c_{ijk} (r, s) is reached.
- 2. Artificial increase of plume σ_y in order to simulate the range of variation of wind direction possible within each wind direction sector.

The advantage of the above approach with respect to conventional climatological models is its ability to take into account preferred segmented plume trajectory patterns induced by complex terrain features, instead of forcing plumes to follow straight lines. Equation 7.1 could also be rewritten to incorporate multihour combined f values, even though the advantages of this second approach may only be apparent.

7.2 Case 2 - Multiple Meteorological Stations

If more than one meteorological station is available (e.g., several surface stations and wind/temperature profiles), Equation 7.1 cannot be applied. In such a case, AVACTA II can still be used in a climatological form, such as

$$\bar{c}(r) = \frac{\sum_{e,m}^{m} f(e,m) c_{e,m}(r) h(e,m)}{\sum_{e,m}^{m} f(e,m) h(e,m)}$$
 (7.2)

where f (e, m) is the measured joint frequency of occurrence, during the period T under examination, of the e-th emission scenario and the m-th meteorological scenario; c_{e, m} (r) is the concentration simulated by AVACTA II in the receptor r of the e-th emission scenario and the m-th meteorological scenario; and h (e, m) is the duration in time of each combined meteorological and emission scenario (e, m).

The use of Equation 7.2 requires:

- 1. The identification of several meteorological scenarios that characterize the area under investigation well (not necessarily a joint combination of wind speed, wind direction and stability) and their typical duration.
- 2. The multi-hour simulation by AVACTA II of c_{e, m} (r), which can be obtained as a steady-state concentration field, assuming the persistence of the e-th emission scenario and the m-th meteorological scenario.
- 3. The artificial increase, as in the previous case, of plume σ_y in order to simulate the possible range of variation of wind direction within each meteorological scenario.

The above scheme may represent a cost-effective solution of the problem if the meteorological scenarios are chosen correctly and if the number of combinations (e, m) is not too high. Some meteorological scenarios can also cover calm or low wind conditions, if appropriate, since AVACTA II is able to simulate these conditions.

The use of a generic meteorological scenariom, instead of the standard classification (i, j, k) described in Section 7.1, allows 1) an easy incorporation of multi-hour cases, and 2) simulations for only the most frequent meteorological conditions.

8. RECOMMENDATIONS FOR POSSIBLE FUTURE ACTIVITIES

This study has provided preliminary results that emphasize the complexity of the dispersion phenomena in the Los Angeles Basin and the need for advanced dispersion modeling techniques to simulate them. Our preliminary runs indicate that dynamic Lagrangian methods (such as AVACTA II) are more accurate than steady-state models and can provide a more realistic assessment of the maximum ground level concentration impact.

We recommend the continuation of this effort with the following tasks:

- o <u>Task 1</u>. Application, calibration and evaluation of AVACTA II against other tracer experiment data in the Southern California.
- o <u>Task 2</u>. Application of more advanced Lagrangian methods, such as our MC-LAGPAR Monte Carlo Lagrangian particle model to available data bases. (Our most recent publication on MC-LAGPAR is enclosed as Appendix H.)
- o <u>Task 3.</u> Implementation and evaluation of the climatological version of AVACTA II, according to the methodologies described in Section 7.

In addition to the possible continuation of this study, as proposed in Tasks 1-3 above, we think that AVACTA II represents an appropriate dispersion tool for an advanced plume visibility model and, therefore, propose the additional task below.

on dispersion formulas that use steady-state straight-line Gaussian plume assumptions. This is a serious limitation that strongly limits the reliability of these packages. We propose to incorporate into AVACTA II the visibility modules developed by Professor Ronald Henry of USC. The goal is to develop, using available computational modules and theories, a plume visibility package with a more realistic description of plume dispersion than currently done.

9. REFERENCES

- Fox, D.G. (1981): Judging air quality model performance. <u>Bull. Amer. Meteor.</u> Soc. 62: 599-609.
- Fox, D.G. (1984): Uncertainty in air quality modeling. <u>Bull. Amer. Meteor.</u> Soc. 65: 27-36.
- Ludwig, F.L., L.S. Gasiorek and R.E. Ruff (1977): Simplification of a Gaussian puff model for real-time minicomputer use. Atmos. Environ. 11: 431-436.
- McElroy, J.L., and F. Pooler (1968): St. Louis dispersion study, Volume 2, Analysis. Department of Health, Education and Welfare, Report AP-53.
- Turner, D.B. (1985): Proposed pragmatic methods for estimating plume rise and plume penetration through atmospheric layers. Atmos. Environ. 19(7): 1215-1218.
- Zannetti, P. (1981): An impoved puff algorithm for plume dispersion simulation.

 J. Appl. Meteor. 20: 1203.
- Zannetti, P., V.S. Perun and M.W. Chan (1981; 1982): AVACTA II: User's Guide -- Release 1. AeroVironment report, AV-FR-81/598 (Release 2, AV-FR-81/598R, 1982).
- Zannetti, P., G. Carboni and R. Lewis (1986): AVACTA II -- User's Guide, Release 3, AeroVironment Report (AV-OM-85/520).
- Zannetti, P., D.M. Wilbur and G.E. Schacher (1982): Characterizing coastal atmospheric diffusion from three-dimensional monitoring of SF₆ releases. Preprint, First International Conf. on Meteorology and Air/Sea Interaction of the Coastal Zone, Amer. Meteor. Soc., Boston, MA.