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MEMORANDUM

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SUBJECT: ESTIMATION OF METHYL ISOTHIOCYANATE AIR CONCENTRATIONS
ASSOCIATED WITH PRIORITY CASE NUMBER 026-KER-05

This memorandum revision changes the name identification of the vineyard where workers experienced symptoms consistent with exposure to methyl isothiocyanate. All references to Sun Pacific are changed to 7th Standard Ranch Company.

I. Background

This modeling analysis was conducted in support of the investigation of the incident 26-KER-05. This incident occurred near Mettler, California. A standard sprinkler application of metam sodium was begun on August 3, 2005 and completed on August 5, 2005. At approximately 0720 hours Pacific Daylight Time (PDT) on the mornings of August 5 and August 6 workers in the 7th Standard Ranch Company grape vineyard north of the treated field reportedly experienced a range of symptoms consistent with methyl isothiocyanate (MITC) exposure. This memorandum provides estimates of both the location of the plume of MITC and the MITC air concentrations in the vicinity of the standard sprinkler application.

II. Methyl Isothiocyanate Air Concentration Estimates

A. Application Parameters

The treatment site is identified on Map Number 1653 generated by the Kern County Agricultural Commissioner's office on July 06, 2005. Map Number 1653, 2005 Map-Permit Number 1501871, shows the Val-Mar treatment site 83A, carrots, 75.4 acres. Location of the 7th Standard Ranch Company grape fields directly to the north is also shown (Figure 1).

The 75.4 acre treatment site was divided into 6 approximately equal 12.5 acre rectangular subsections (Figure 2). Each subsection was treated separately, one sprinkler set per subsection and five sprinkler lines per set. The reported treatment/follow-up watering-in (water seal) schedule is shown in Table 1. According to the Notice of Intent to apply Restricted Materials, the treatment site was treated with Sektagon 42[®] at a rate of 45 gal/acre. This product contains 4.22 lbs



metam sodium/gal. It will be assumed for this analysis that there is a 100% conversion of metam sodium to the active ingredient MITC.

B. Meteorological Conditions

There are no meteorological stations closer than approximately 14 miles from the site of 26-KER-05. Therefore, to characterize the likely wind conditions on the mornings of August 5 and 6, meteorological data were obtained from five stations in the general Bakersfield area (Figure 3). Two types of meteorological station data were available: California Irrigation Management Information System (CIMIS) and California Air Resources Board Air Quality and Meteorological Information System (AQMIS). It should be noted that the Arvin-Edison CIMIS station (#125) and the Arvin-Bear Mountain Boulevard AQMIS station are located about 0.25 miles apart on the Arvin-Edison Water Storage District offices property. Tables 2 and 3 show the wind conditions and air temperatures recorded at these meteorological stations during 0600 hours to 0800 hours PDT on the mornings of August 5 and 6, 2005.

C. Methyl Isothiocyanate Flux Estimates

Flux estimates provided by Wofford (2005) for a night-time sprinkler application (Wofford et al., 1994) were used to approximate the 26-KER-05 application MITC flux. Proportional adjustments were made to the Wofford (2005) flux estimates to account for product and application rate differences. The Wofford et al. (1994) study used the product Vapam[®] with 32.7% (3.18 lb/gal metam sodium) at a rate of 100 gal/acre. Two adjustments to the Wofford (2005) flux estimates are necessary to match the 26-KER-05 application:

1. $(4.22 \text{ lb/gal}) / (3.18 \text{ lb/gal}) = 1.327$
2. $(45 \text{ gal/acre}) / (100 \text{ gal/acre}) = 0.45$

Therefore, total adjustment to Wofford (2005) flux estimates is $1.327 * 0.45 = 0.5972 \sim 0.6$. The resulting adjusted flux estimates are shown in Table 4.

The Wofford (2005) MITC flux estimates are the best available estimates. However, it is not known how well these flux estimates match the true flux at the 26-KER-05 application site at the time of the incidents. The Wofford (2005) flux estimates were obtained by the back-calculation method (Ross et al., 1996) and the regression fits were quite good (see analysis in Wofford, 2005). Therefore, the flux estimates themselves have relatively low variance. However, since Wofford (1994) is the only existing study of a night-applied standard sprinkler application, the magnitude of between-application variance is unknown. Thus, it is not possible to quantify the uncertainty introduced by using the flux profile from Wofford (2005) to estimate air concentrations associated with 26-KER-05 incident. However, it is known from data for other fumigants that flux estimates for similar application methods can vary by as much as 50% (Barry, 1999).

D. Air Dispersion Modeling

The U.S. Environmental Protection Agency (U.S. EPA) Industrial Source Complex Model Short Term (ISCST3) (U.S. EPA, 1995) was used to estimate air concentrations associated with the sprinkler application. Flux estimates were chosen from those shown in Table 4 to match the timing of the applications and the incidents. The flux estimates selected for the simulations are shown in Table 5.

1. Source Geometry

August 5. For the morning of August 5, 2005, the field was represented by three sources (Figure 4). The first source contained the three subsections of the field (one half the total area) that were treated August 3 to 4. The second source contained the two 12.5 acre subsections that were applied the night of August 4 (2000-2330 hours PDT) and early the morning of August 5, (0000-0330 hours PDT). The third source contained the 12.5 acre subsection that was applied from 0400-0600 hours PDT the morning of August 5. The flux estimates used for the August 5, 2005, simulation are shown in Table 5 and the ISCST3 input file is shown in Appendix A.

August 6. For the morning of August 6, 2005 the field was divided approximately in half to represent the three subsections applied on August 3 to 4 as one source and the three subsections applied on August 4 to 5 as a second source. For simulation purposes it was assumed that enough time had elapsed since the application that the three subsections in the same half of the field were emitting MITC at the same rate. Thus, the field may be represented by two sources and the same flux estimate can be used for the three subsections in each source. The source layout is shown in Figure 5 and the flux estimates used are shown in Table 5 and the ISCST3 input file is shown in Appendix A.

2. Stability Class and Wind Speed Specification

August 5. On August 5, 2005, sunrise was at 0608 hours PDT. Thus, the atmospheric conditions between 0600 hours and 0800 hours were in transition from night to day. The incident on August 5, 2005, occurred between 0615 hours and 0720 hours PDT. During this time it is possible that a surface inversion was present but it would have been in the process of breaking up as time after sunrise progressed (Schnelle and Dey, 2000). Stability class F was assigned to the 0600–0700 hour PDT. U.S. EPA procedure is to change only one atmospheric stability class per hour (U.S. EPA, 1999). In addition, when assigning stability class, dark hours are considered to be one-hour following sunrise, in this case 0708 hours PDT. Atmospheric conditions were beginning to cycle toward daytime during the 0700–0800 hours PDT. However, ongoing light wind conditions, low solar radiation and low sun angle all suggest the potential for persistent stable atmospheric conditions at the beginning of the first hour following sunrise (0700–0800 hours PDT). For these reasons, stability F was chosen to characterize atmospheric stability and produce modeling

scenarios. Light wind speeds throughout the area suggested a wind speed of 1m/s for all modeling scenarios.

August 6. On August 6, 2005, sunrise was at 0609 hours PDT. Thus, as on August 5, the atmospheric conditions between 0600 hours and 0800 hours were in transition from night to day. The incident on August 6, 2005 also occurred between 0615 hours and 0720 hours PDT. During this time it is possible that a surface inversion was present but it would have been in the process of breaking up as time after sunrise progressed (Schnelle and Dey, 2000). Stability class F was assigned to the 0600–0700 hour PDT. U.S. EPA procedure is to change only one atmospheric stability class per hour (U.S. EPA, 1999). In addition, when assigning stability class, dark hours are considered to be one hour following sunrise, in this case 0709 hours PDT. Atmospheric conditions were beginning to cycle toward daytime during the 0700–0800 hours PDT. However, ongoing light wind conditions, low solar radiation and low sun angle all suggest the potential for persistent stable atmospheric conditions at the beginning of the first hour following sunrise (0700–0800 hours PDT). For these reasons, stability F was chosen to characterize atmospheric stability and produce modeling scenarios. Light wind speeds throughout the area suggested a wind speed of 1m/s for all modeling scenarios.

3. Wind Direction Uncertainty Analysis

Two methods were used to account for wind direction uncertainty at the treatment site during the August 5, 2005 incident. The uncertainty is due to the distance to the closest weather station (approximately 14 miles) and the low wind speed conditions at and immediately following sunrise.

Simulate a range of wind directions. The first method to account for wind direction uncertainty was to simulate a range of wind directions based upon observations at the four AQMIS stations meteorological stations. The Arvin-Edison CIMIS station was removed from this analysis because the wind directions measured at that station were not consistent with the AQMIS stations. To characterize the potential location of the plume during the 0700-0800 hours on August 5 and August 6, wind directions representing the outer ranges and the midpoint of the directions observed each day at the four AQMIS stations were used as input to the ISCST3 model. For August 5, wind directions (“to” or plume centerline direction) of 248°, 292°, and 270° were used to produce concentration isopleth maps. For August 6, wind directions (“to” or plume centerline direction) of 291°, 328°, and 310° were used to produce concentration isopleth maps.

Estimate spatial uncertainty of the Arvin-Edison CIMIS Station predicted plume centerline location. The second method used a technique developed by Sajo (2003) to estimate spatial uncertainty associated with the Arvin-Edison CIMIS Station predicted plume centerline. Details are described in Appendix B. This technique uses the standard deviation of horizontal wind direction (σ_θ) to calculate bounds on the plume centerline location. The calculated bounds

allow comparison of the potential range of the Arvin-Edison CIMIS station predicted centerline with the plume centerlines predicted by the four AQMIS stations.

IV. Results and Discussion

A. ISCST3 Simulations

1. August 5

Plume location. Figures 6 through 8 show ISCST3 results for the range of wind directions simulated as part of the uncertainty analysis (248° , 292° , and 270°). These results indicate that the range of wind directions reported during the 0700–0800 hours PDT on August 5, 2005, results in plumes mostly oriented away from the 7th Standard Ranch Company Grapes site. However, the AQMIS Edison and Bakersfield-Golden State Highway stations both report wind directions that would produce plume centerline directions (292° and 288° , respectively) causing the plume of MITC emitting from the Val-Mar application site to contact the workers in the 7th Standard Ranch Company Grapes site. The spatial uncertainty bounds calculated for the Arvin-Edison CIMIS station allow for the plume centerline direction to have been as far northwest as 285° (see Appendix B). These results indicate it is reasonable to conclude that on the morning of August 6, the plume of MITC emitting from the Val-mar application site contacted the workers in the 7th Standard Ranch Company Grapes site.

Magnitude of MITC air concentrations. Estimated 1-hr time weighted average (TWA) MITC air concentrations in the plume potentially contacting workers at the 7th Standard Ranch Company Grapes site are approximately 0.50 ppm. The peak-to-mean adjusted air concentrations for 30 minute, 10 minute, and 3 minute TWA are shown in Table 6. The estimated short-term peak concentrations vary between 0.65 ppm for the 30 minute average and 2.00 ppm for the 3 minute average. These peak-to-mean adjusted air concentrations are according to Hino (1968) and Turner (1994) as described in Barry (2000).

2. August 6

Plume location. Figures 9 through 11 show ISCST3 results for the range of wind directions simulated as part of the uncertainty analysis (291° , 328° , and 310°). These results indicate it is reasonable to conclude that during 0700–0800 hours PDT on August 6, 2005, the plume of MITC emitting from the Val-Mar application site contacted the workers in the 7th Standard Ranch Company Grapes site. In addition, the spatial uncertainty bounds calculated for the Arvin-Edison CIMIS station allow for the plume centerline direction to have been as far northwest as 306° (see Appendix B). These results indicate it is reasonable to conclude that on the morning of August 6 the plume of MITC emitting from the Val-mar application site contacted the workers in the 7th Standard Ranch Company Grapes site.

Magnitude of MITC Air Concentrations. Estimated 1-hr TWA MITC air concentrations in the plume potentially contacting site near the reservoir in the 7th Standard Ranch Company Grapes site varied between 0.05 ppb and 0.15 ppb. The peak-to-mean adjusted air concentrations for 30 minute, 10 minute, and 3 minute TWA are shown in Table 6. The estimated short-term peak concentrations in the vicinity of the workers vary between 0.06 ppm for the 30 minute average and 0.60 ppm for the 3 minute average. These peak-to-mean adjusted air concentrations are according to Hino (1968) and Turner (1994) as described in Barry (2000).

B. Uncertainty in the Magnitude of Estimated MITC Air Concentrations

Air concentrations estimated by the ISCST3 model are directly proportional to the flux used to obtain the estimates. For methyl bromide Barry (1999) found a coefficient of variation of 50% in back-calculated flux studies for similar application methods. Qualitatively applying this field-to-field variability to the MITC flux implies an uncertainty range of approximately double for the flux estimates used in all six simulations. Uniformly doubling the flux would double the air concentrations shown in Figures 6-11.

C. MITC Air Concentration Estimates in the Context of Effects Levels

Odor threshold estimates for MITC range over an order of magnitude or more. Alexeef et al. (1994) give the odor threshold for MITC as a range from 0.1–5 ppm, citing Nesterova (1969) and Verschueren (1983). It is not clear how the 0.1 ppm lower bound was estimated. However, Verschueren (1983) clearly cites the odor threshold as 4.93 ppm. Verschueren (1983) states that the odor threshold is the 50% Recognition Threshold defined as: “. . . the concentration at which 50% of the odor panel defined the odor as being representative of the odorant being studied.” The odor threshold is essentially an instantaneous value. The Gaussian Plume model algorithm is generally agreed to produce air concentration estimates on the order of 10 minute to 60 minute averages. ISCST3 model estimates in this memorandum are essentially 1-hr (60 minutes) TWA concentrations because the time scale of the concentration estimate is related to the averaging time of the weather data used to obtain the estimate. AQMIS and CIMIS weather data are 1-hr TWA observations. Shorter-term concentration estimates were obtained by using peak-to-mean estimation techniques (Barry, 2000). These techniques use adjustment factors derived from analysis of field studies investigating the patterns of air concentrations measured in the same pollutant plume over a range of averaging times to scale a 1-hr TWA concentration estimate to shorter time interval estimates. Table 6 presents estimates of shorter averaging periods for estimated concentrations along the 1-hr TWA isopleths using the peak-to-mean techniques.

A human subject study examining effects of MITC exposure was completed by Russell and Rush (1996). Ruben (2002), in an evaluation of MITC as a toxic air contaminant, reports that the observed odor threshold for MITC in the Russell and Rush (1996) study showed a range of 0.2 to 8 ppm with a geometric mean of 1.7 ppm. These odor threshold bounds overlap with those from the earlier MITC odor threshold evaluations. However, the range is even larger than that cited by Alexeef et al. (1994). The fact that the odor threshold can vary over more than an order of magnitude between individuals has important implications for both the analysis of incidents such as this one and also the detection of conditions requiring odor mitigation associated with metam sodium applications. Individual response is highly variable.

Ruben (2002) also summarized the eye irritation responses observed in the Russell and Rush (1996) study. A one to two hour constant exposure to 0.8 ppm of MITC resulted in an eye irritation response in the majority of test subjects. Thus, Ruben (2002) reports LOEL (lowest observed effect level) as 0.8 ppm. NOEL (no observed effect level) for eye irritation was 0.2 ppm. Positive eye irritation responses were also observed at both 1.9 ppm and 3.3 ppm for 4 and 14 minutes of exposure. Respiratory irritation was not characterized because respiratory exposure was not part of the Russell and Rush (1996) study.

V. Conclusion

These results indicate it is reasonable to conclude that on the mornings of August 5 and August 6, 2005, the plume of MITC emitting from the Val-mar application site contacted the workers in the 7th Standard Ranch Company Grapes site. The location of the plumes shown in Figures 6 through 11 should not be interpreted as the exact location of the plumes at any particular moment during the incidents. With regard to area sources and peak-to-mean estimates, Best et al. (2002) state: “. . . area sources show non-zero concentrations on the centerline for virtually all of the time, but still with a high degree of variability.” Therefore, it should be kept in mind that the plume shifts back and forth over a general area over shorter time periods, on the order of minutes to one hour. Plume centerlines as shown in the figures are mean locations as characterized by the weather data used to obtain the estimates. Air concentrations at any particular spot over a short time period (peak concentration estimates) are potentially significantly higher than the 1-hr TWA concentrations. In this context, the magnitude of MITC concentrations may be uncertain but the concentration isopleths shown in Figures 6–11 and the peak concentration estimates shown in Table 6 indicate that air concentrations at the site of the incidents could reasonably have been within the range of MITC concentrations associated with odor and eye irritation responses as summarized by Ruben (2002).

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Table 1. Reported schedule of Vapam 42[®] metam sodium treatment and follow watering in (water seal). See Figure 2 for site diagram and identification of treatment subsections.

Treatment Subsection	Treatment		Water Seal	
	Date	Time (hours)	Date	Time (hours)
1	08/03/05	2000-2330	08/04/05	1000-1130
2	08/04/05	0000-0330	08/04/05	1200-1330
3	08/04/05	0400-0600	08/04/05	1500-1630
4	08/04/05	2000-2330	08/05/05	1000-1130
5	08/05/05	0000-0330	08/05/05	1200-1330
6	08/05/05	0400-0600	08/05/05	1500-1630

Table 2. Meteorological data from six stations in the Bakersfield area for the critical hours 0600 and 0800 PDT on August 5, 2005. See Figure 3 for the location of these stations relative to the treatment site.

Station	0600 hours–0700 hours				0700 hours–0800 hours			
	Air Temperature (C)	“From” Wind Direction (degrees)	“To” Wind Direction (degrees)	Wind Speed (m/s)	Air Temperature (C)	“From” Wind Direction (degrees)	“To” Wind Direction (degrees)	Wind Speed (m/s)
CIMIS Arvin (125)	21.7	73.9	253.9	0.89	25.6	42.7	222.7	0.72
AQMIS Arvin-Bear Mountain Boulevard	26.1	86	266	0.55	27.2	68	248	1.0
AQMIS Edison	22.8	105	285	2.1	26.1	112	292	2.1
AQMIS Bakersfield-5558 California Avenue	23.9	110	290	0.55	25.0	102	282	1.0
AQMIS Bakersfield-Golden State Highway	24.4	85	265	0.89	25.6	108	288	1.8

Table 3. Meteorological data from six stations in the Bakersfield area for the critical hours 0600 and 0800 PDT on August 6, 2005. See Figure3 for the location of these stations relative to the treatment site.

Station	0600 hours–0700 hours				0700 hours–0800 hours			
	Air Temperature (C)	“From” Wind Direction (degrees)	“To” Wind Direction (degrees)	Wind Speed (m/s)	Air Temperature (C)	“From” Wind Direction (degrees)	“To” Wind Direction (degrees)	Wind Speed (m/s)
CIMIS Arvin (125)	24.4	59.7	239.7	0.94	27.8	51.5	231.5	0.95
AQMIS Arvin-Bear Mountain Boulevard	27.8	98	278	1.03	28.9	144	324	0.54
AQMIS Edison	26.1	97	277	2.60	27.8	135	315	1.56
AQMIS Bakersfield-5558 California Avenue	25.0	73	253	1.03	26.1	111	291	1.03
AQMIS Bakersfield-Golden State Highway	26.1	127	307	1.34	27.2	148	328	1.79

Table 4. Flux estimates for the 26-KERN-05 incident. These estimates were derived using flux estimates from a night sprinkler application as reported by Wofford (2005). The adjustment factor is 0.6. See text for derivation of the adjustment factor.

Event	Wofford (2005) flux ($\mu\text{g}/\text{m}^2\text{sec}$)	26-KERN-05 flux ($\mu\text{g}/\text{m}^2\text{sec}$)
Application (night)	486	292
1 st Night–6 hours	191	115
1 st Day–6 hour	24.7	14.8
1 st Day–6 hours	34.0	20.4
2 nd Night–12 hours	34.4	20.6
2 nd Day–12 hours	4.2	2.5
3 rd Night–12 hours	3	1.8

Table 5. Flux estimates for the sources used in the ISCST3 input files for the mornings of August 5 and 6, 2005. Note that Source A and Source D represent the same portion of the field and Source E consists of Sources B and C together.

August 5	
Source	Flux
A	20.4 $\mu\text{g}/\text{m}^2\text{sec}$
B	115.0 $\mu\text{g}/\text{m}^2\text{sec}$
C	292.0 $\mu\text{g}/\text{m}^2\text{sec}$
August 6	
Source	Flux
D	1.8 $\mu\text{g}/\text{m}^2\text{sec}$
E	20.4 $\mu\text{g}/\text{m}^2\text{sec}$

Table 6. Peak-to-mean adjusted ISCST3 1-hr TWA MITC air concentration (ppm) estimates.

	Isopleth Air Concentration (ppm)					
Peak Interval	0.05	0.15	0.20	0.30	0.40	0.50
30 minute	0.06	0.20	0.26	0.39	0.52	0.65
10 minute	0.11	0.34	0.46	0.69	0.92	1.15
3 minute	0.20	0.60	0.80	1.20	1.60	2.00

Figure 1. Kern County Agricultural Commissioner office map of the Val-Farms site, 2005 Permit Number 1501871. Note: That the block labeled "Sun Pacific's Grapes" is the 7th Standard Ranch Company site.

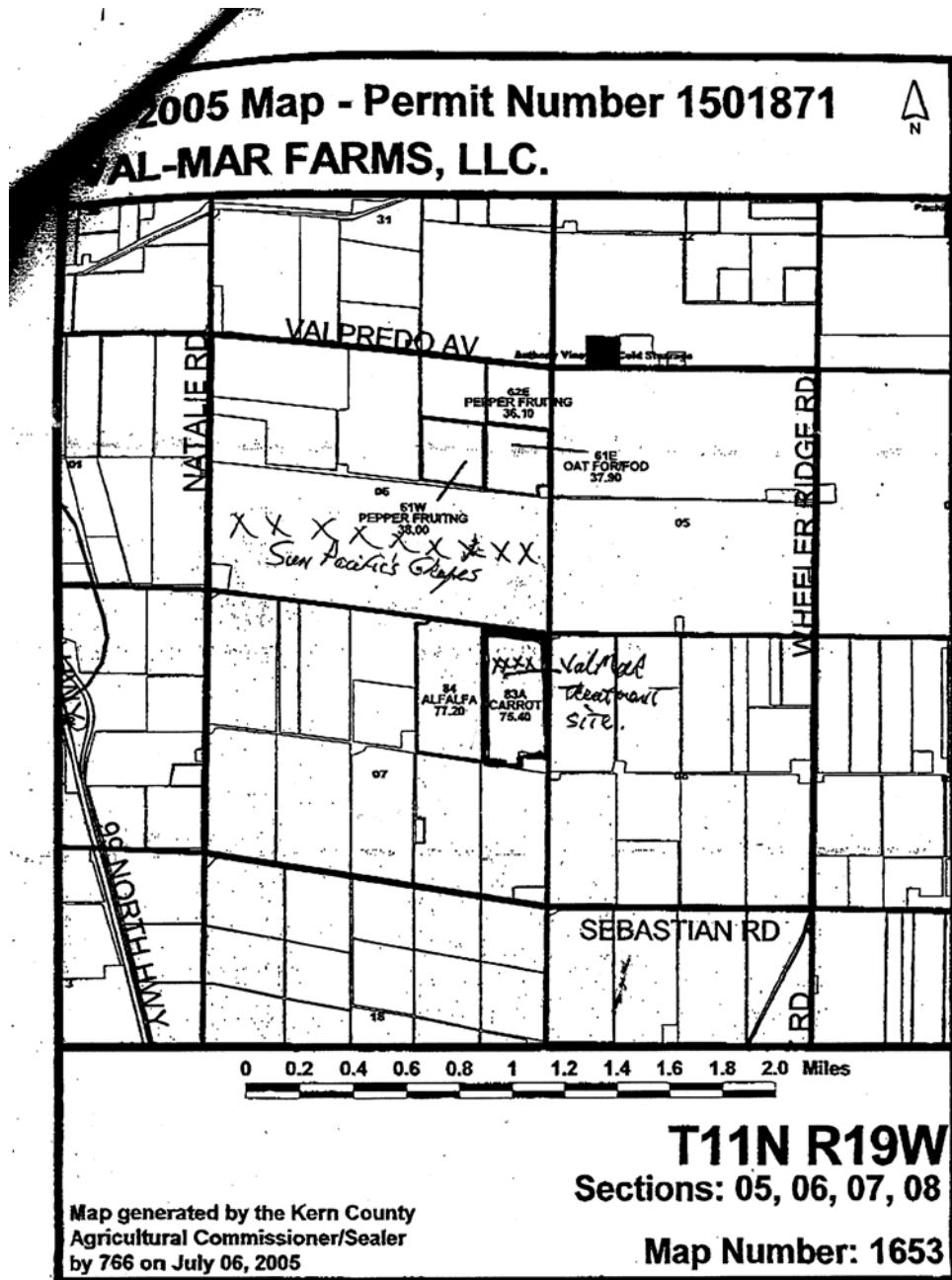


Figure 2. Val-Mar Farms site map indicating the subsections (sprinkler sets) and order of application. Note: That the dirt road labeled "Sun Pacific side" is the 7th Standard Ranch Company site.

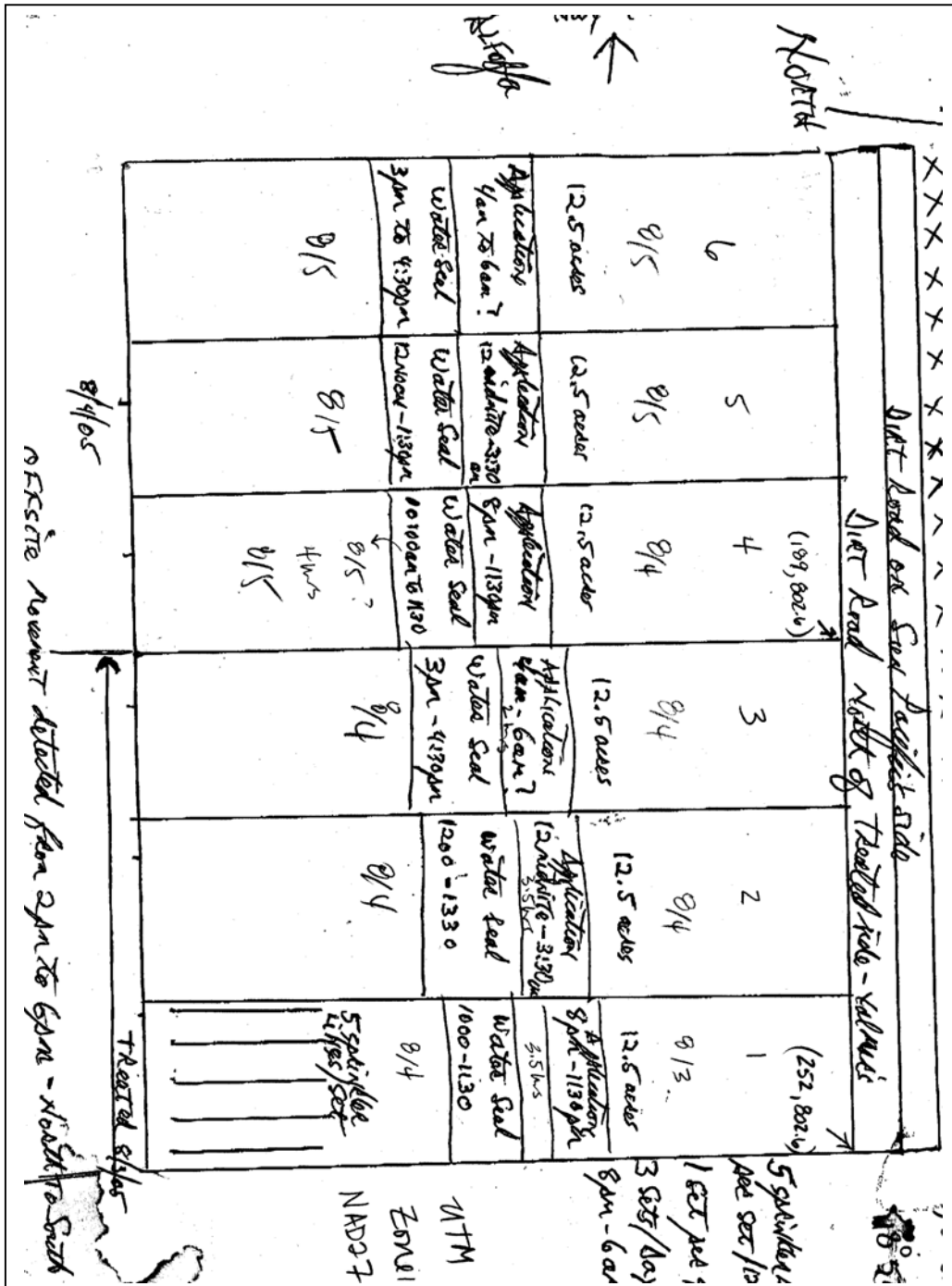


Figure 3. Locations of the five weather stations in the Bakersfield area relative to the Val-Mar Farms application site.

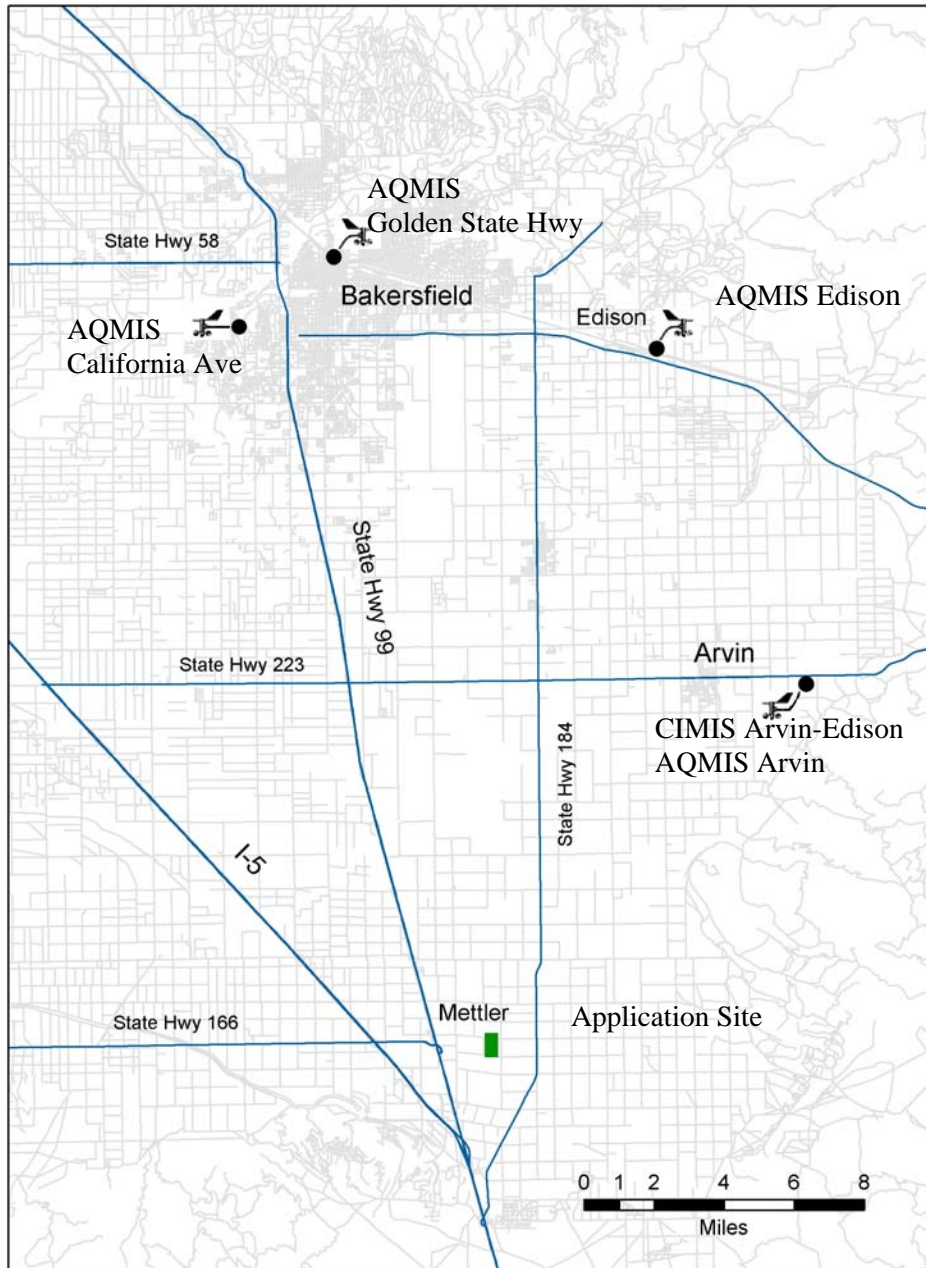


Figure 4. Source geometry, flux estimates, and receptor locations used for the August 5, 2005, ISCST3 simulation. Map is in Teale-Albers coordinants. Units on the x and y axes are meters. Location of work crew is noted.

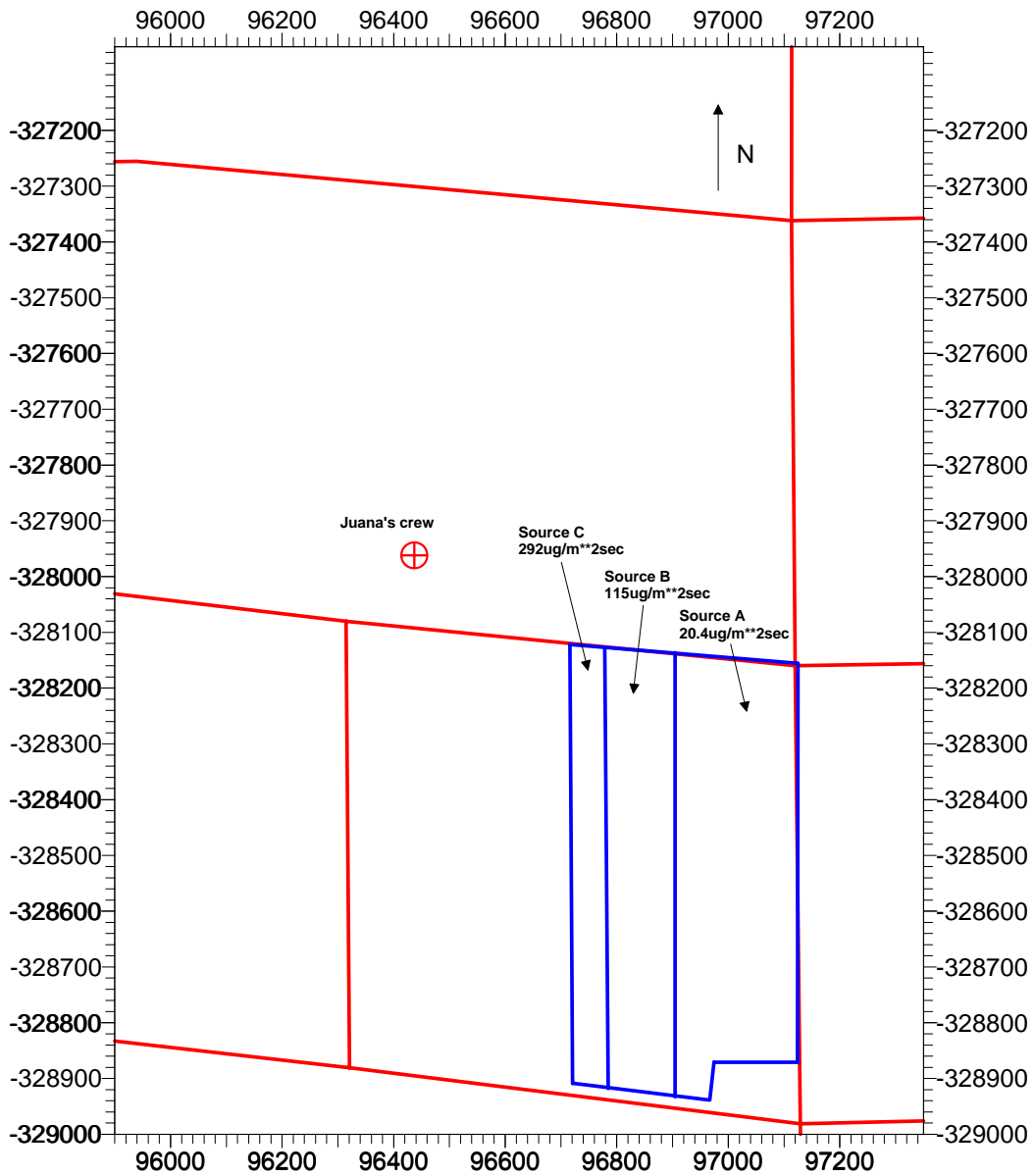


Figure 5. Source geometry, flux estimates, and receptor locations used for the August 6, 2005, ISCST3 simulation. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.

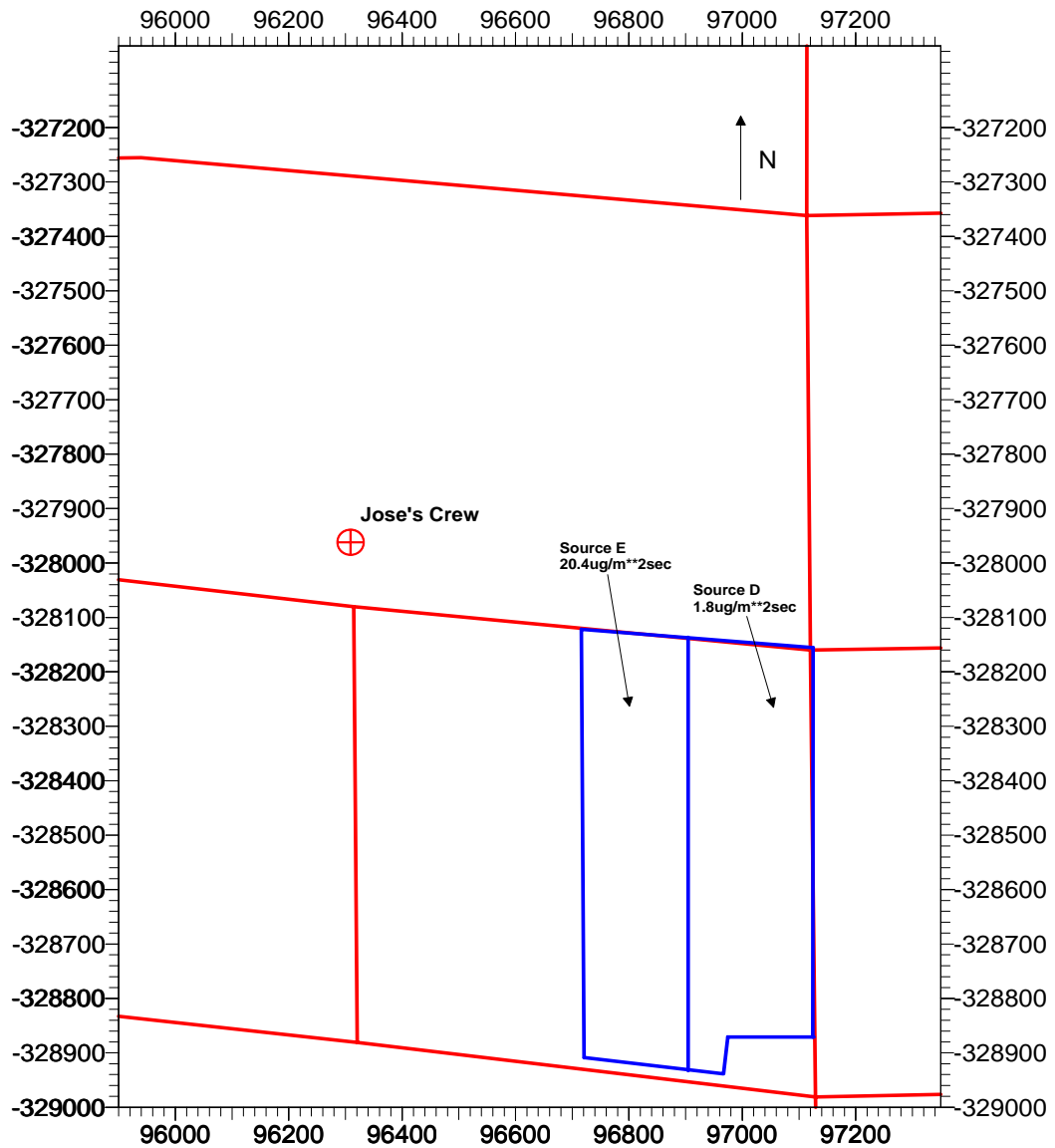


Figure 6. Methyl isothiocyanate concentration isopleths (ppm), August 05, 2005, 0700–0800 hours PDT. Weather data input: 248° plume centerline direction, 1 m/s wind speed, F-stability. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.

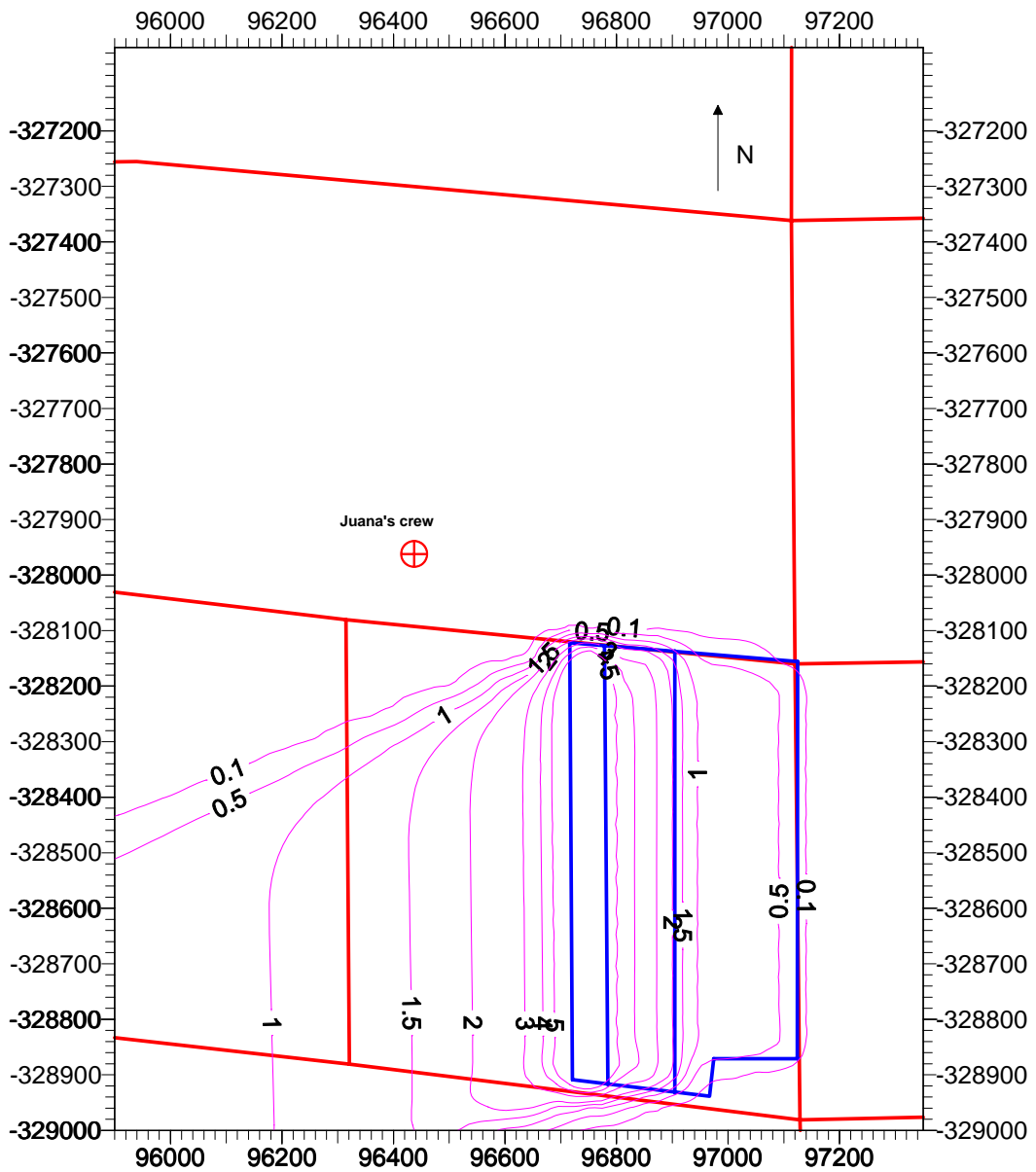


Figure 7. Methyl isothiocyanate concentration isopleths (ppm), August 05, 2005, 0700–0800 hours PDT. Weather data input: 270° plume centerline direction, 1 m/s wind speed, F-stability. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.

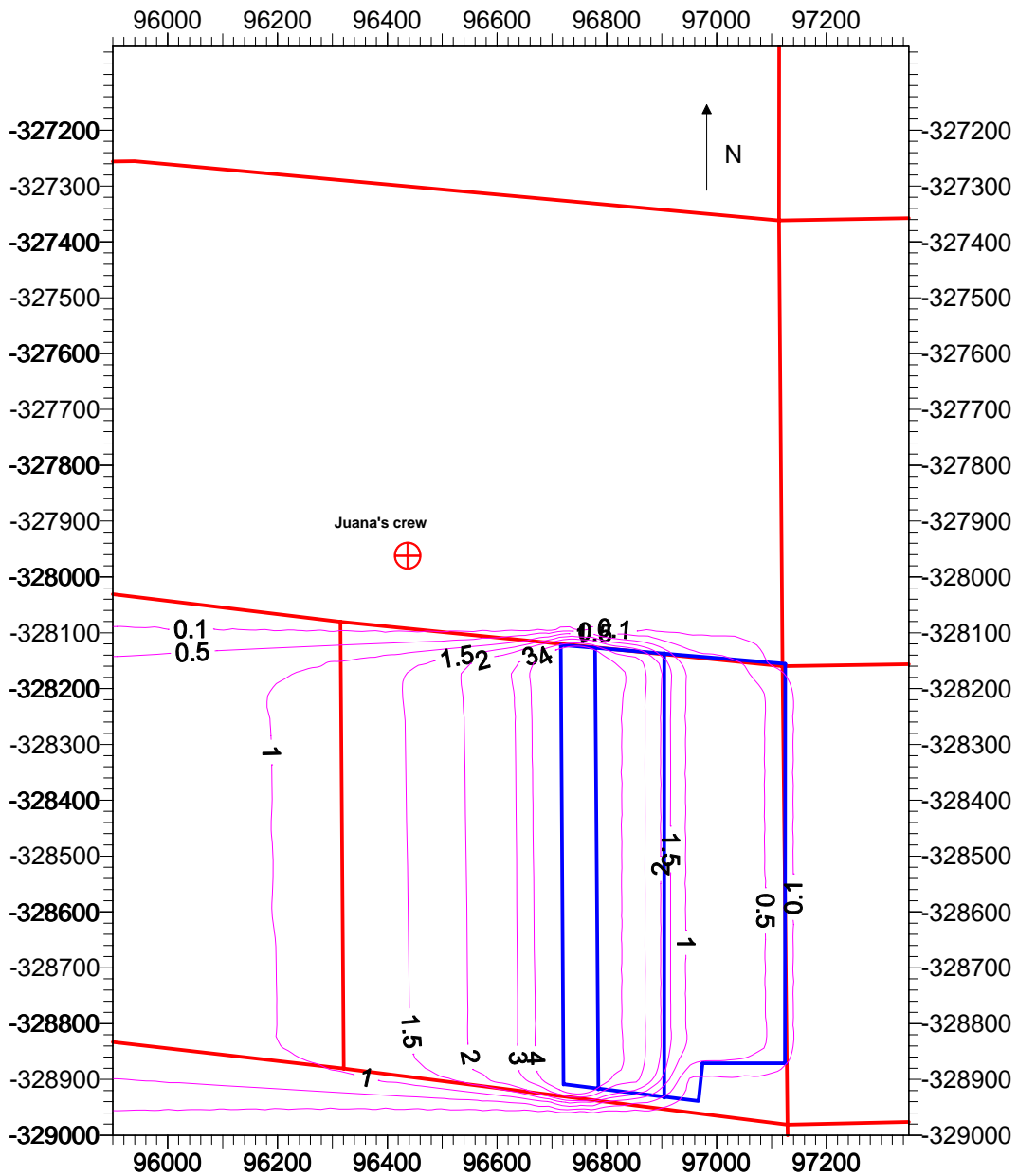


Figure 8. Methyl isothiocyanate concentration isopleths (ppm), August 05, 2005, 0700–0800 hours PDT. Weather data input: 292° plume centerline direction, 1 m/s wind speed, F-stability. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.

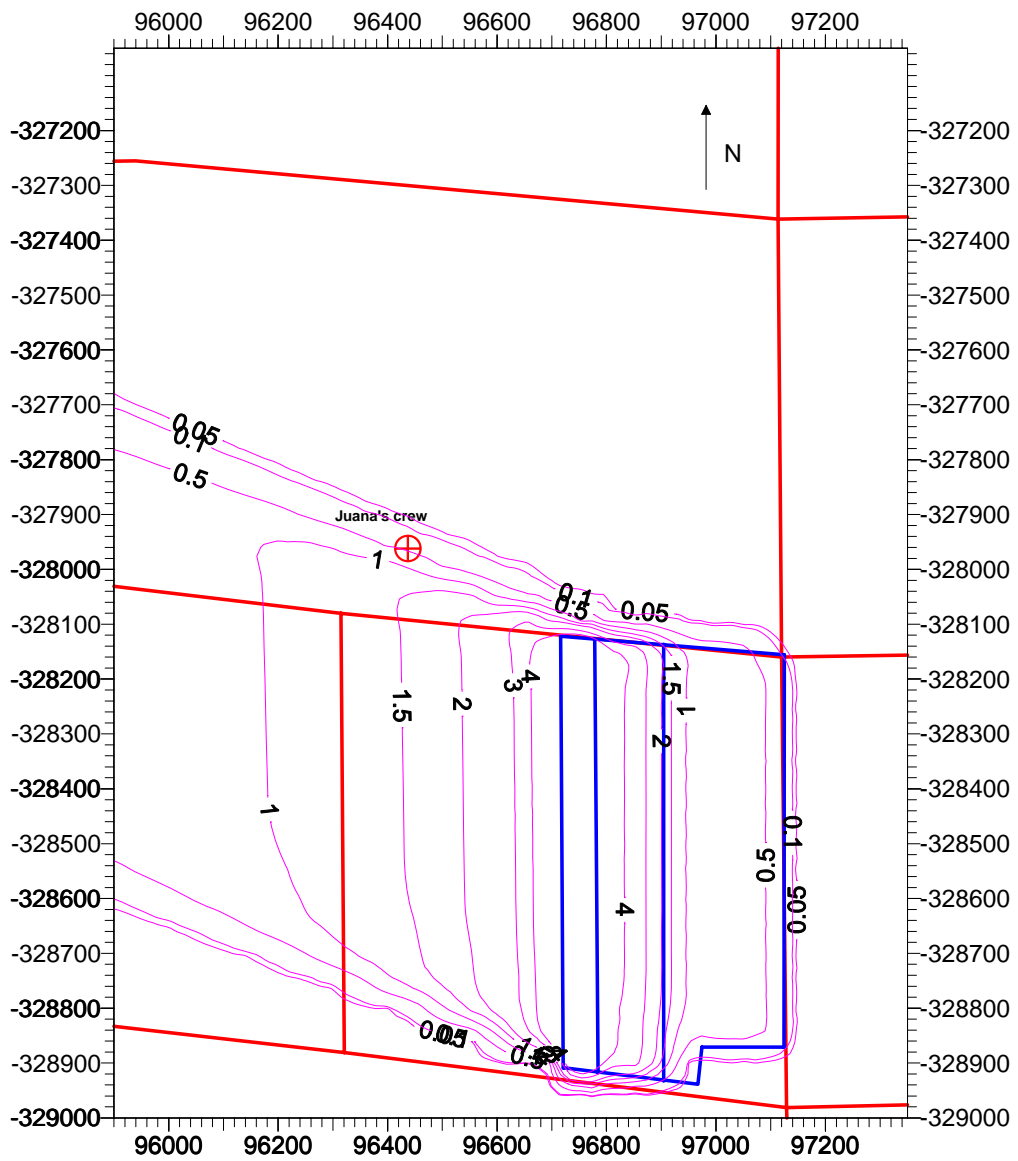


Figure 9. Methyl isothiocyanate concentration isopleths (ppm), August 06, 200, 0700–0800 hours PDT. Weather data input: 291° plume centerline direction, 1 m/s wind speed, F-stability. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.

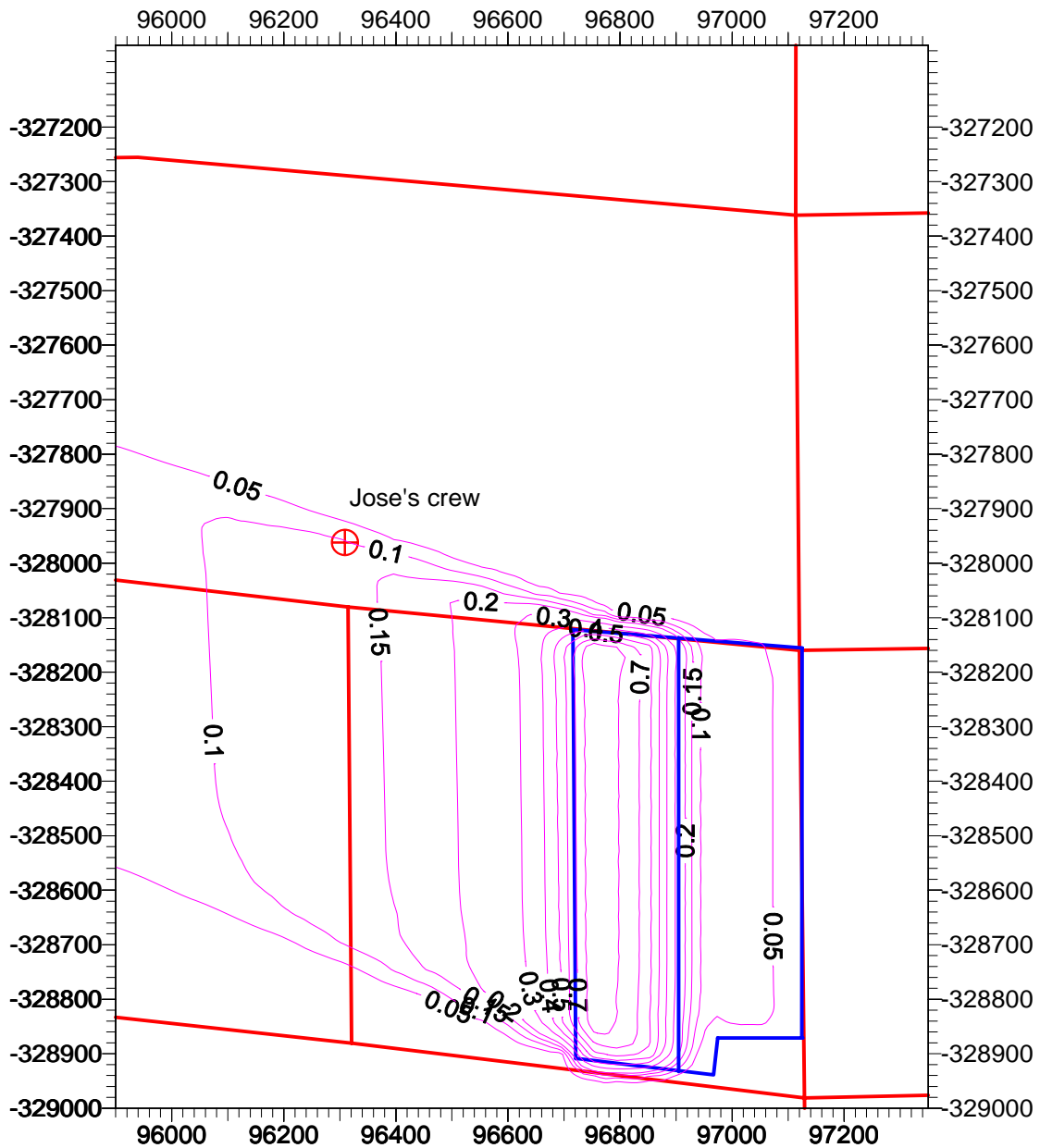


Figure 10. Methyl isothiocyanate concentration isopleths (ppm), August 06, 200, 0700–0800 hours PDT. Weather data input: 310° plume centerline direction, 1 m/s wind speed, F-stability. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.

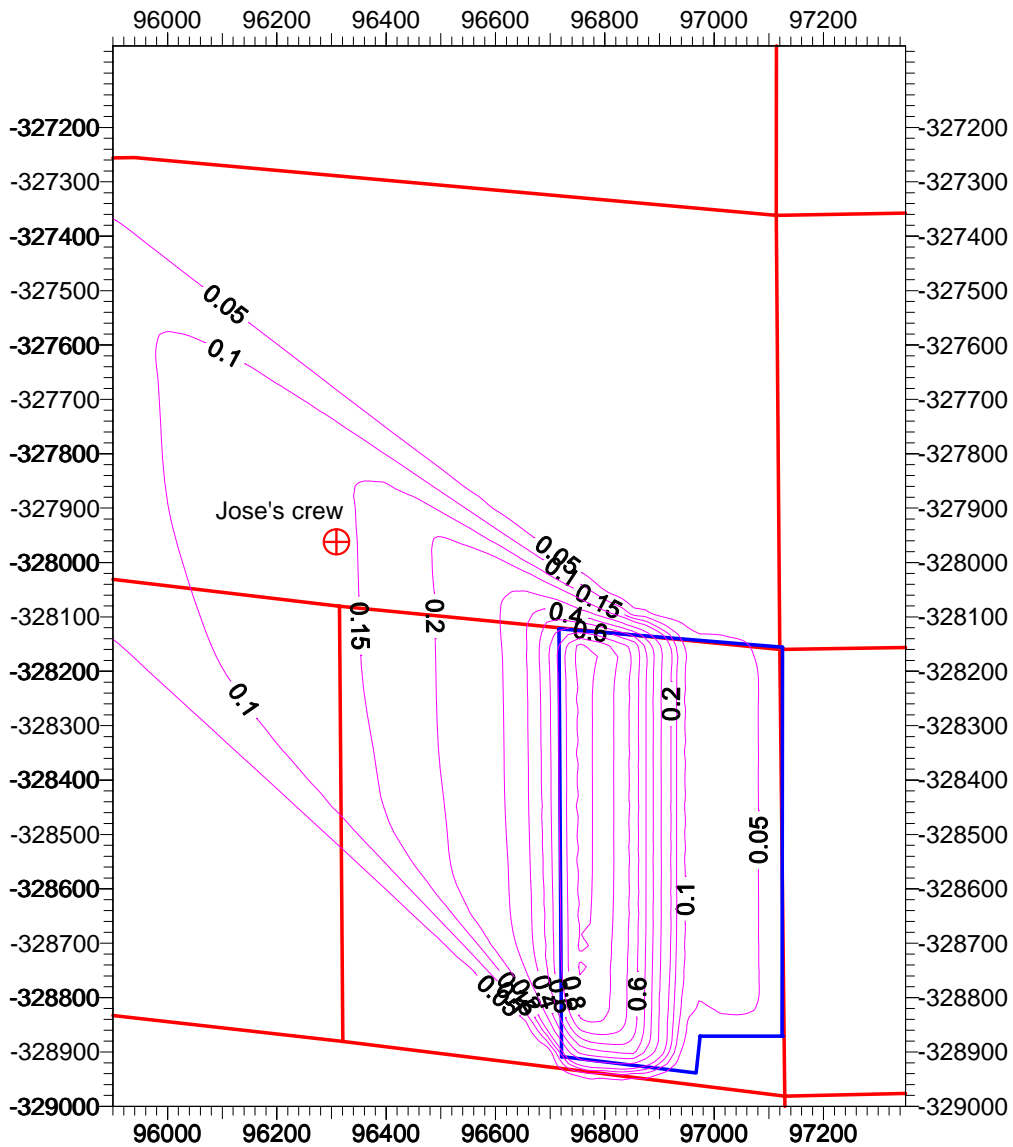
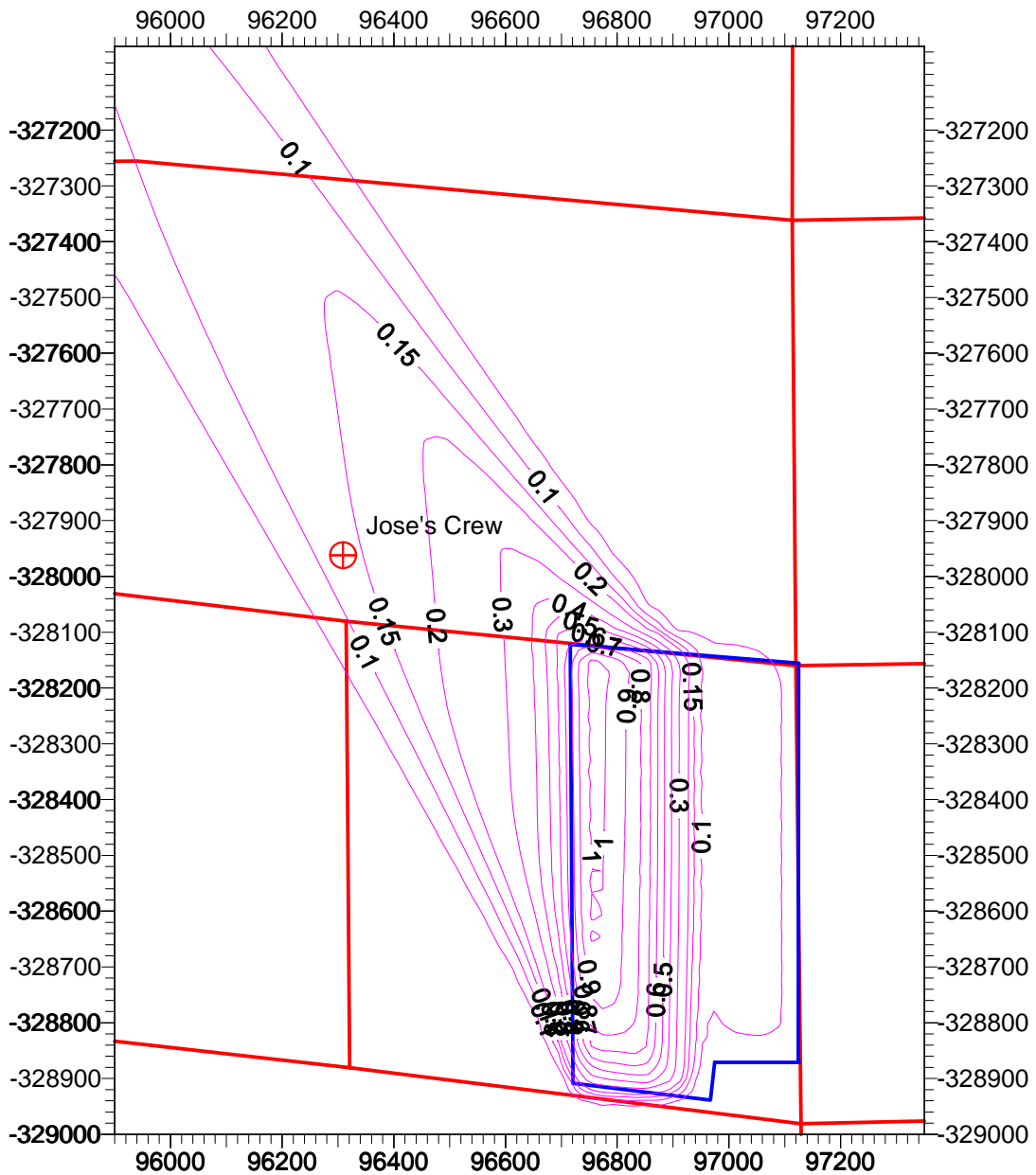


Figure 11. Methyl isothiocyanate concentration isopleths (ppm), August 06, 2005, 0700–0800 hours PDT. Weather data input: 328° plume centerline direction, 1 m/s wind speed, F-stability. Map is in Teale-Albers coordinates. Units on the x and y axes are meters. Location of work crew is noted.



Kean S. Goh, Ph.D.
November 30, 2005
Page 25

Appendix A

ISCST3 Input file for August 5, 2005

```
CO STARTING
CO TITLEONE MetamSodium 26-KER-05 8/6 0700-0800
CO MODELOPT CONC RURAL NOSTD NOBID NOCALM
CO AVERTIME period
CO POLLUTID OTHER
CO DCAYCOEF .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FINISHED
SO STARTING
** Source Location Cards:
** SRCID SRCTYP XS YS ZS
SO LOCATION 1 AREAPOLY 96974.0 -328871.00 0.0000
SO LOCATION 2 AREAPOLY 96905.75 -328931.50 0.00
SO LOCATION 3 AREAPOLY 96784.0 -328917.0 0.00
SO LOCATION 4 AREAPOLY 96722.0 -328909.00 0.00
** Source Parameter Cards:
** AREA: SRCID QS HS NVERT
SO SRCPARAM 1 .020400000E-03 .0000 4
SO AREAVERT 1 96974.0 -328871.00 96967.0 -328135.7
1 97125.0 -328156.0 97126.0 -328871.0
SO SRCPARAM 2 .020400000E-03 .0000 4
SO AREAVERT 2 96905.75 -328931.50 96905.75 -328137.4
2 96967.0 -328137.7 96974.0 -328871.0
SO SRCPARAM 3 .115000000E-03 .0000 4
SO AREAVERT 3 96784.0 -328917.00 96778.0 -328127.0
3 96905.75 -328137.4 96905.75 -328931.5
SO SRCPARAM 4 .292000000E-03 .0000 4
SO AREAVERT 4 96722.0 -328909.00 96716.0 -328122.0
4 96778.0 -328127.00 96784.0 -328917.0
SO EMISUNIT .100000E+07 (GRAMS/SEC) (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED
RE STARTING
RE GRIDCART CAR STA
RE GRIDCART XYINC 95900.00 30 50 -329000.00 40 50
RE GRIDCART CAR END
RE FINISHED
ME STARTING
ME INPUTFIL aug0505w.txt (4I2,2F9.4,F6.1,I2,2F7.1)
ME ANEMHGHT 10.000 METERS
ME SURFDATA 99999 2005 SURFNAME
ME UAIRDATA 99999 2005 UAIRNAME
ME WINDCATS 1.54 3.09 5.14 8.23 10.80
ME FINISHED
OU STARTING
OU PLOTFILE PERIOD ALL aug0505.plt
OU FINISHED
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ISCST3 Input file for August 6, 2005

```
CO STARTING
CO TITLEONE MetamSodium 26-KER-05 8/6 0700-0800
CO MODELOPT CONC RURAL NOSTD NOBID NOCALM
CO AVERTIME period
CO POLLUTID OTHER
CO DCAYCOEF .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FINISHED
SO STARTING
** Source Location Cards:
** SRCID SRCTYP XS YS ZS
SO LOCATION 1 AREAPOLY 96974.0 -328871.00 0.0000
SO LOCATION 2 AREAPOLY 96905.75 -328931.50 0.00
SO LOCATION 3 AREAPOLY 96722.0 -328909.00 0.00
** Source Parameter Cards:
** AREA: SRCID QS HS NVERT
SO SRCPARAM 1 .0018000000E-03 .0000 4
SO AREAVERT 1 96974.0 -328871.00 96967.0 -328135.7
1 97125.0 -328156.0 97126.0 -328871.0
SO SRCPARAM 2 .0018000000E-03 .0000 4
SO AREAVERT 2 96905.75 -328931.50 96905.75 -328137.4
2 96967.0 -328137.7 96974.0 -328871.0
SO SRCPARAM 3 .0204000000E-03 .0000 4
SO AREAVERT 3 96722.0 -328909.00 96716.0 -328122.0
3 96905.75 -328137.4 96905.75 -328931.5
SO EMISUNIT .100000E+07 (GRAMS/SEC) (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED
RE STARTING
RE GRIDCART CAR STA
RE GRIDCART XYINC 95900.00 30 50 -329000.00 40 50
RE GRIDCART CAR END
RE FINISHED
ME STARTING
ME INPUTFIL aug0605w.txt (4I2,2F9.4,F6.1,I2,2F7.1)
ME ANEMHGHT 10.000 METERS
ME SURFDATA 99999 2005 SURFNAME
ME UAIRDATA 99999 2005 UAIRNAME
ME WINDCATS 1.54 3.09 5.14 8.23 10.80
ME FINISHED
OU STARTING
OU PLOTFILE PERIOD ALL aug0605.plt
OU FINISHED
```

Kean S. Goh, Ph.D.
November 30, 2005
Page 28

Appendix B

Spatial Uncertainty Estimation

The Sajo (2003) technique requires an estimate of the standard deviation of horizontal wind direction (σ_θ). This technique uses the standard deviation of horizontal wind direction (σ_θ) to calculate bounds on the plume centerline location. Amongst the five meteorological stations, only the Arvin-Edison CIMIS station recorded σ_θ . The calculated bounds allow comparison of the potential range of the Arvin-Edison CIMIS station predicted centerline with the plume centerlines predicted by the four AQMIS stations.

On August 5, the σ_θ estimates were 18 degrees and 39.5 degrees for 0600–0700 hours PDT and 0700–0800 hours PDT, respectively. On August 6, the σ_θ estimates were 35.1 degrees and 74.6 degrees for 0600–0700 hours PDT and 0700–0800 hours PDT, respectively. The doubling in σ_θ between 0600–0700 hours PDT and 0700–0800 hours PDT observed both mornings likely reflect either the presence of meander conditions or the process of transition between night and day. The effect of meander is not addressed by the Sajo (2003) method. Meander tends to occur on clear nights under very light wind speeds. In this case the standard deviations of wind direction for one-hour can be very large. However, this does not reflect turbulence. Rather, it reflects the slower back-and-forth movement of the plume. During meander conditions, the mean wind direction reported may not reflect the predominant direction over the hour or there may not have been a predominant direction. The process of transition from night to day consists of a shift in atmospheric conditions from the stable conditions at night to less stable conditions during the day. Atmospheric conditions become more turbulent as the ground heats after sunrise. The increase in solar radiation between 0600–0700 hours and 0700–0800 hours supports the premises that the more likely condition associated with the doubling in σ_θ is transition between night and day. In that case the Sajo (2003) method may be applied.

The Sajo (2003) technique was applied to the Arvin-Edison CIMIS 0700–0800 hours PDT meteorological data for both August 5 and 6. This method yields a confidence interval on the centerline plume direction using the Arvin-Edison CIMIS meteorological data. To use this method values must be specified for two measures of uncertainty associated with the dispersion model ensemble mean concentrations. These two measures of uncertainty are the factor of validity, n , and the logarithmic standard deviation of the local concentration (σ_l). The factor of validity is a function of σ_θ , y_0 (crosswind location), and the confidence level (Ci) and provides an upper and lower bound on the actual concentration at a location given the model computed ensemble mean (e.g. $\chi(x_0, y_0) = n(Ci)\bar{\chi}(x_0, y_0)$, where $\bar{\chi}(x_0, y_0)$ = model ensemble mean predicted concentration at location (x_0, y_0)). In this analysis $y_0 = 0$ because only the uncertainty in the location of the centerline will be estimated. Model uncertainty, and thus the value of n , can vary widely depending upon the conditions under which the predictions are made. Hanna (1982)

has placed model uncertainty between 2 and 10. Miller and Hively (1987) report for ground level sources under low wind speed conditions predicted-to-observed ratios of 1 to 100 and $\sigma_l = 1.77$ (geometric standard deviation = $\sigma_g \sim 6$). Van der Hoven (1981) has characterized the predicted-to-observed ratio for ground-level releases under low wind speed conditions as about an order of magnitude (a factor of 10). In practice, n and σ_g are often assumed to have the same value (Sajo, per. comm., 2005).

The equations needed to estimate the spatial uncertainty are shown below:

$\Delta\theta = \frac{1}{2}$ width of the confidence interval on the plume centerline (radians)

$$\Delta\theta = \tan^{-1}(\sigma_\theta \sqrt{G(n, \sigma_l)}) \quad (1)$$

Where:

$$G(n, \sigma_l) \equiv -\sigma_l^2 \pm \sqrt{4 \ln^2(n) + 12\sigma_l^2 \ln(n) + \sigma_l^4} = \text{scaling parameter} \quad (2)$$

Only the positive solution for $G(n, \sigma_l)$ has physical meaning (Sajo, 2003).

The confidence interval is:

$$\text{Centerline} \pm \Delta\theta$$

For the estimation of spatial uncertainty on both August 5 and 6, a value of $n = 10$ will be used because σ_θ is large on both days. The large σ_θ suggests that $\sigma_g > 6$ (Sajo, per. comm., 2005).

Therefore, a value of $\sigma_g = 7$ will be used for the estimates. The spatial uncertainty bounds will have approximately a 97% confidence level. The estimates for both cases are shown below. Calculations are performed in radians, results are shown in degrees. See Sajo (2003) for details and theory regarding derivation of the estimates.

August 5

$$n = 10$$

$$\sigma_g = 7 \Rightarrow \sigma_l = 1.95$$

$$\sigma_\theta = 39.5^\circ = 0.6894 \text{ radians}$$

plume centerline direction = 222.7°

$$G(n, \sigma_l) \equiv -\sigma_l^2 \pm \sqrt{4 \ln^2(n) + 12\sigma_l^2 \ln(n) + \sigma_l^4}$$

$$G(10, 1.95) = -(1.95)^2 \pm \sqrt{4 \ln^2(10) + 12(1.95)^2 \ln(10) + (1.95)^4} = 8.05$$

$$\Delta\theta = \tan^{-1}(0.6894\sqrt{8.05}) = 1.101 \text{ radians} = 63.1^\circ$$

Bounds on plume centerline spatial uncertainty = $222.7^\circ \pm 63.1^\circ = (159.6^\circ, 285.8^\circ)$

Thus, the Arvin-Edison CIMIS meteorological data produces, with ~97% confidence, a centerline direction for the MITC plume emitting from the application during 0700–0800 hours PDT on August 5 that lies between approximately 160° and 286° .

August 6

$$n = 10$$

$$\sigma_g = 7 \Rightarrow \sigma_l = 1.95$$

$$\sigma_\theta = 74.6^\circ = 1.302 \text{ radians}$$

plume centerline direction = 231°

$$G(n, \sigma_l) \equiv -\sigma_l^2 \pm \sqrt{4 \ln^2(n) + 12\sigma_l^2 \ln(n) + \sigma_l^4}$$

$$G(10, 1.95) = -(1.95)^2 \pm \sqrt{4 \ln^2(10) + 12(1.95)^2 \ln(10) + (1.95)^4} = 8.05$$

$$\Delta\theta = \tan^{-1}(1.302\sqrt{8.05}) = 1.3064 \text{ radians} = 74.8^\circ$$

Bounds on the plume centerline spatial uncertainty = $231^\circ \pm 74.8^\circ = (156.2^\circ, 305.8^\circ)$

Kean S. Goh, Ph.D.
November 30, 2005
Page 32

Thus, the Arvin-Edison CIMIS meteorological data produces, with ~97% confidence, a centerline direction for the MITC plume emitting from the application during 07000–0800 hours PDT on August 6 that lies between approximately 156° and 306° .