Department of Pesticide Regulation

MEMORANDUM

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SUBJECT: ANALYSIS OF 1,3-DICHLOROPROPENE EMISSIONS FOR FIELD ONE IN THE LOST HILLS STUDYCONSIDERING HIGH FLUX DENSITIES FROM THE BARE GROUND NEAR THE TARP EDGE

Background

Gao et al. (2013) measured flux using a dynamic flux chamber on and near the edge of a fumigant application. The application was 587 lbs/acre Pic-Chlor which consists of 60% chloropicrin and 40% 1,3-dichloropropene (1,3-d) to an 8 acre field (Ajwa and Sullivan 2012). A totally impermeable film ([TIF], "VaporSafe" TM, Raven Industries) covered the field. Gao et al. (2013) reported measurements next to tarp edge which were an order of magnitude higher than corresponding flux measurements over the tarp. Their tarp edge flux measurements were also an order of magnitude larger than the tarp fluxes estimated by back-calculation (Ajwa and Sullivan 2012). Farther out at 2m from tarp edge, Gao et al. (2013) reported nearly zero measured flux. Simulation with HYDRUS2D/3D of gas movement for this application was consistent with high flux in the untarped zone adjacent to the covered field (Spurlock et al. 2013, Figure 2). The HYDRUS2D/3D model also predicted an exponential decline with distance away from the tarp edge, consistent with the very low flux Gao et al. (2013) reported at 2m from the tarp edge. Wang et al. (2010) found measurable soil gas concentrations of 1,3-d and chloropicrin up to 6m away from the edge of a virtually impermeable film (VIF) tarp covering a shanked application. The presence of a fumigant gas in the soil atmosphere is obviously a precondition for surface flux and is consistent with flux from the untarped region next to a tarped fumigant application.

The back-calculation technique for estimating flux depends on comparing ISCST3 (U.S. EPA 1995) model simulations to offsite air concentration measurements period by period in order to estimate flux. A key element in this procedure is the proportional relationship between concentration and flux embodied in the Gaussian equation. Historically, the tarped field alone has been represented as a source. In the case of the Lost Hills Study (Ajwa and Sullivan 2012), the field was a single, approximately 8 acre source. Laboratory measurements of tarp permeability for the TIF tarp utilized in the Lost Hills Study estimate a mass transfer coefficient under ambient conditions of <0.0000 cm/h for either 1,3-d or chloropicrin (Qian et al. 2011).

Thus, the high fluxes from the untarped field margins reported by Gao et al. (2013) together with the laboratory-measured tarp impermeability (Qian et al. 2011) suggest the extreme possibility that the dominant contributions to concentrations measured by offsite air monitors were from the tarp margins with very little contribution from the tarped field itself.

The aim of this work is to simulate the eight acre Lost Hills field using ISCST3 with both field and margin flux sources in order to determine the relative contribution from both sources and what difference, if any, potential margin flux makes to off-site air monitor concentrations.

Specifically, the questions are:

1. How well do the Gao et al. (2013) fluxes estimate the monitored results when used in ISCST3 and compared to the measured offsite air concentrations?
2. What differences are there between ISC estimated monitor concentrations based on (1) tarp flux source only, (2) margin flux sources only, and (3) margin plus tarp flux sources.
3. Does adding the margin area flux sources improve back-calculation regression analysis, especially for periods when the initial regression was not significant?
4. Is it possible based on the regression analysis to conclusively determine if the monitored air concentrations result from (1) tarp flux source only, (2) margin flux sources only, and (3) a combination of tarp and margin flux sources.
5. Is it possible that actual flux through the tarp is zero, consistent with laboratory-measured flux values, and air concentrations monitored by offsite pumps were due solely to flux from the edge of the tarps?

Methods

The field representation for the purposes of ISCST3 modeling that was used by Ajwa and Sullivan (2012) was a polygon with four vertices in UTM coordinates (Figure 1). The field was not a perfect square, but nearly so. In order to simulate a margin around the field, it was necessary to approximate the margin with a series of rectangles. A requirement for rectangular area sources is that the length to width ratio is 10 or less (U.S. EPA, 1995 pages 3-35). In order to enable flexibility in setting the margin width for ISCST3 control files, two steps were taken: (1) the field was approximated by a perfect square and corner coordinates were simplified and (2) a computer program was written to create a list of sources covering the margin and satisfying the 10:1 ratio requirement. The computer program required a square field.

Periods 5,6,7,8 and the fumigant 1,3-d were selected for simulation. These periods were each 6 hours long, had measureable offsite air concentrations and two periods (6,8) with initially significant back-calculation regressions and two periods with non-significant back-calculation regressions. The first goal was to compare the back-calculation flux density estimates based on the idealized square field geometry to those based on the original polygon geometry. As long as differences were small, then the following work could proceed. For convenience, the original 16 discrete receptor locations were transformed by subtracting 256000m and 3926000m from the east-west and north-south UTM coordinates, respectively. This resulted in 3 digit location coordinates. The idealized field was represented within this transformed coordinate system. The 16 discrete receptors were located at alternating distances of 10m and 20m distances from the field.

I obtained 1,3-d flux data from Suduan Gao (personal communication) which was the basis for Gao et al. (2013) and was taken in parallel to the offsite air monitoring for Field 1 in the Lost Hills Study. It was necessary to establish a correspondence between the timing of the flux measurements and the off-site air monitoring periods in order to utilize Gao et al. (2013) flux for each of the periods 5-8 which I studied.

Once the flux measurements from Gao et al. (2013) were aligned with the offsite measurement periods, the Gao et al. (2013) fluxes were inserted into ISCST3 to estimate the monitored air concentrations. These estimates were compared to the measured air concentrations.

Further ISCST3 simulations were conducted to explore the relationships between measured 1,3-d concentrations and various source combinations and will be described in subsequent sections.

Results

Idealized square field representation

The original control files (Ajwa and Sullivan 2012) used the AREAPOLY and AREAVERT keywords (see example in Appendix). The modified control file representing the idealized field used the LOCATION keyword. The idealized field coordinates were used in ISCST3 simulations to estimate 1,3-d concentrations at the monitors and regress the measured concentrations on these ISCST3 estimates. For this set of ISCST3 simulations the only flux source was the tarped field. There was no flux from untarped field edge. The purpose was to test the similarity in results between the original analysis and this new analysis with the idealized field coordinates representing a square.

These revised back-calculation regression with the idealized field coordinates gave results that were very similar to the original analyses (Table 1). There were small differences in slopes and intercepts. Consequently, utilizing a square field did not have any important effect on estimation of the flux for periods 5-8. For these four periods, there were two periods where the regressions were significant (6,8) and two periods where the regression were not significant (5,7).

The similarity of the results from the two geometries is reinforced by directly comparing the estimated concentrations at each monitor location (Table 2). These simulations were performed by utilizing the same flux (1ug/m2s) and meteorological input with only the geometries slightly different: one was the original polygon geometry and the other was the idealized perfect square representation of the field. The slopes and nearly perfect r2 values suggest a 1:1 relationship between the two sets of estimated concentrations. Therefore, the idealized field geometry gave results that were so close to the actual field geometry results that resultant ISCST3 simulations will be relevant to the original field.

A FORTRAN computer program was written to facilitate the creation of the ISCST3 control files for the margin sources (MARGINS01.FOR). The program along with example input and output files are listed in the Appendix. The output from this program was used to construct ISCST3 control files which used two source groups: the on field tarped area and the untarped sources representing a 0.5m (50cm) wide margin around the field (Figure 2). The width of 50cm was chosen because the dynamic flux chambers measured 51cm x 25cm (Qin et al. 2011) and were oriented perpendicular to the tarp edge (Gao et al. 2013). Distinguishing these two source groups enables requesting ISCST3 concentration estimates based on each source group separately and combined within a single simulation. The margin source group consisted of 152 individual sources 50cm wide and with various lengths created to cover the margin around the field constrained so that the length to width ratio was less than or equal to 10. The idealized field was 181m x 181m with a 50cm wide zone around the edge. The idealized tarped field area was 32761m2 and the untarped margin zone area was (181.5m x 0.5m) x 4=363m2.

Aligning Monitoring Periods

The monitoring periods from Gao et al. (2013) were aligned with the offsite air concentration monitoring periods (Table 3). This resulted in two flux estimates for periods 5 and 7 and one flux estimate each for periods 6 and 8. The two flux estimates were averaged for the period. The side by side comparison of flux densities shows that the Gao et al. (2013) on-tarp flux estimates were higher than those derived from the back-calculation procedure (Table 4). In periods 7 and 8, the chamber-measured tarp fluxes were 3 to 4 times higher than those derived from back-calculation.

Concentration estimates using Gao et al. (2013) flux measurements

The fluxes from Gao et al (2013) were used in ISCST3 to estimate the monitor concentrations under three combinations: tarp flux only (margin flux set to zero), margin flux only (tarp flux set to zero), and tarp and margin flux. The resulting concentration estimates were averaged for the 16 monitors and compared to the measured concentration average. The ISCST3 estimates based on only flux from the margin were closest to the average measured concentrations (Figure 3). The ISCST3 concentration estimates based on both the margin and tarp fluxes from Gao et a. (2013) overestimated the measured concentrations in periods 5,7,8. ISCST3 estimated concentrations based only on the measured tarp flux from Gao et al. (2013) were approximately similar to measured concentrations in periods 5 and 6, but overestimated measured concentrations for periods 7 and 8.

The fact that these ISCST3 estimates are higher than the measured concentrations does not a priori distinguish between two possible explanations: (1) ISCST3 concentration estimates are too high or (2) Gao et al. (2013) flux measurements are too high. Model bias is possible. Systematic differences have been found in comparing ISCST3 to AERMOD, for example. This shows that models of this kind may be biased. ISCST3 generally estimates higher concentrations than AERMOD for point sources (Hall et al. 2000, Long et al. 2004). For area sources ISCST3 also appears to estimate generally higher concentrations. Schroeder (2004) found 88% of ISCST3 estimates were higher than their corresponding AERMOD estimates over a grid using area sources for five years of data. I obtained the data from Schroeder (Schroeder personal communication) and regressed AERMOD results on ISCST3 results for the annual comparison and found a multiplicative constant of 0.78. This result is very close to the 0.72 I found in comparing ISCST3 annual estimates to AERMOD annual estimates using Parlier 2006 meteorology and a gridded set of receptors (Johnson, 2013). Shorter time periods such as in the current study, however, produced much greater variability in ISCST3 to AERMOD comparisons. It may be possible to assess model bias by comparing ISCST3 back-calculated flux densities to directly measured flux densities when both are conducted in a single field study. On the other hand, the dynamic flux chamber method may be subject to biases. Previous difficulties with this measurement technique involved localized temperature effects (Yates et al. 1996); pressure differentials (Reichman and Ralston 2002); or moisture accumulation (Gao 2010).

Laboratory permeability measurements for this kind of TIF tarp show nearly immeasurable low mass transfer coefficients for 1,3-d. Dynamic flux chamber field measurements on the same kind of TIF tarp in a different study showed peak emission fluxes for 1,3-d of 1.3 (1.0) ug/m2s on the continuous portion of the tarp and 8.0 (13.2) ug/m2s on the glued portion (mean, sd, Qin et al. 2011). When the maximum possible MTC of 0.00004 cm/h is used with the maximum under-tarp air concentration measurements on the order of 10 ug/cm3 (Gao et al. 2013) to estimate flux, a flux density of 0.001 ug/m2s is the result (see Appendix for details). This is three orders of magnitude lower than any of the field-based flux measurements. Thus, dynamic flux chamber measurements on the TIF tarp in the field measure report a flux density not possible based on the laboratory measurements of TIF permeability. Gao et al. (2013) conducted laboratory permeability measurements on fresh and field-used TIF from the Lost Hills study. They found that post-study 1,3-d mass transfer rate was about 3 orders of magnitude larger than pre-study mass transfer rate (Gao et al. 2013, their Table 1). These insights suggest that the behavior of TIF in the field is not the same as in the laboratory and that despite extraordinarily low laboratory-measured mass transfer coefficients, TIF in the field exhibits greater permeability.

The dynamic flux chambers use an inlet air source located 3m above the soil surface. This could create a sampling artifact–showing measured flux when there was none. According to Gao et al. (2013), “The fresh air inlet (sourced from 3m above soil surface via a PVC pipe) to each chamber was continuously sampled for background corrections.” The magnitude of these corrections is not reported but the concentrations are low in comparison to the chamber concentrations (Gao personal communication). This implies that the inlet sources would only potentially be a source of minor error in the chamber measurements and field measured fluxes through TIF material is a real phenomenon.

For each period, I regressed the 16 measured offsite monitor concentrations on the ISCST3 concentration estimates which utilized Gao et al. (2013) flux densities. In using ISCST3 there were three cases. I estimated monitor concentrations using (1) only the tarp flux source (no margin flux), (2) only the margin flux sources (no tarp flux), and (3) both tarp and margin flux sources (Table 5). Only period 6 and 8 yielded significant regressions for measured concentrations regressed on ISCST3 estimated concentrations. In both periods all three source combinations gave statistically significant results. The pattern of significant periods was the same as the pattern found in Ajwa and Sullivan (2012), where periods 6 and 8 yielded significant initial regressions, whereas periods 5 and 7 did not. The strength of the tarp only and margin only regressions flip-flopped in comparing periods 6 and 8. In period 6, the r2 for tarp was 0.48 compared to 0.83 for margin. However, it was 0.83 compared to 0.46 for tarp and margin in period 8. Thus, there was no strong improvement in regressions favoring any of the three possible source sets.

The last column in Table 5 clearly demonstrates the entanglement of tarp- and margin-based concentration estimates. In this column, the ISCST3 concentration estimates based on the margin flux reported in Gao et al. (2013) were regressed on the ISCST3 concentration estimates based on the tarp flux reported in Gao et al. (2013). For each period, the regression was significant. Since the slope was less than 1.0 for all four periods (0.83, 0.3, 0.12, 0.40), the contribution from tarp flux was generally greater (though the flux was much lower), than the contribution from the margin flux (though the flux was much higher). The area of the margin as a fraction of the tarped area was on the order of 1%. But the margin area is closer to the monitors and the flux may be much higher than the tarped field. For each period, the ISCST3 model uses the same meteorology to calculate the area concentrations. This set of physical relationships leads to the entanglement of the margin and tarp fluxes in terms of their effect on estimated monitor concentrations.

Because of the correlated relationship between margin flux and tarp flux based ISCST3 concentration estimates, it is difficult to disentangle the two.

Fraction of ISCST3-estimated monitor concentration due to margin sources

The margin to tarp flux ratio from the fluxes in Table 4 are 55.3, 42.3, 19.1, and 58.1 for periods 5-8, respectively. The average of these four values is 43.8. Keeping this ratio constant through these four periods and setting up an ISCST3 calculation using both tarp and margin fluxes enables a calculation of the margin source contribution to the monitor concentrations under the varying meteorology for these four periods.

The fraction of the estimated monitor concentration due to the margin sources, when the ratio of margin flux to tarp flux was fixed at 43.8 to 1, was 0.40 (0.15), 0.58 (0.26), 0.39 (0.16), and 0.42 (0.19) for periods 5-8 (mean, [standard deviation] over the 16 receptors). Thus under this assumption, the margin sources contribute roughly 1/3 to ½ of the concentrations estimated at the monitor locations. The monitors were located approximately 10-20m from the field. This ratio may be different for receptors farther from the field.

Practical Implications

To gauge the practical effect of high margin sources, the monitor concentrations were estimated using fluxes from Ajwa and Sullivan (2012) and using fluxes from an analysis which used both tarp and margin sources. The latter methodology needs more explanation. The average ratio of margin flux to tarp flux of 43.8 based on the work of Gao et al., (2013) was used to simulate each of periods 5-8. The measured monitor values were regressed on the ISCST3 estimated monitor values (which embodied the 43.8:1 margin: tarp flux ratio). If the regression was significant, the slope was used as the factor to adjust both the assumed tarp and margin flux densities. If the regression was not significant, the mean measured concentration divided by the mean modeled concentration was used as the adjustment factor (Table 6). This operation provided flux adjustment factors which could be used to estimate the monitor concentrations.

The monitor estimates from Ajwa and Sullivan (2012) were then regressed on the ISCST3 monitor estimates based on the 43.8 to 1 margin to tarp flux ratios (Table 6) in order to determine if inclusion of the margin sources in the ISCST3 modeling process made a substantive difference in the monitor concentration estimates.

The regressions for the four periods were all highly significant (Table 7). The slopes were approximately 1. For period 2, the slope of 0.76 fell outside a 95% confidence interval. However, a multi-test error rate for four tests is $1-(0.95)^4=0.19$, so that the result of 1 out of 4 confidence limits excluded 1 not conclusive. The implication is that whether the underlying model includes high margin sources or not, the net monitor concentration estimates will be approximately the same.

Another relevant question is if the high marginal fluxes are a real phenomenon, how much is the tarp flux increased in order to account for the measured monitor concentrations when the margins are not included in the source contributions? To answer this question I simulated each period using the 43.8 to 1 ratio of margin to tarp flux density and obtained the receptor-estimated concentrations based on (1) only the tarp source, (2) only the margin source, and (3) both tarp and margin sources. Within each period, I found the average over the receptors of concentrations for (1) only the tarp source. (2) only the margin source, and (3) both tarp and margin sources. I calculated the ratio between (3) divided by (1) for each period. These ratios were 1.7, 1.7, 1.5 and 1.5 for periods 5-8, respectively. So that under these assumptions, not including the margin flux in the estimate for field flux results in about a 60% increase in the apparent tarp flux in order to make up for the margin sources. For context, this 60% increase is small relative to the difference between the unused and post-field used TIF permeability measurements which showed a three order magnitude increase in the MTC (Gao et al. 2013).

Conclusion

Measurement of flux on the tarp and on the soil immediately adjacent to the tarp resulted in high flux densities during a TIF tarp study (Gao et al. 2013). Measurement and soil diffusion modeling indicated that these high fluxes tapered off rapidly away from tarp edge. An ISCST3 control file was developed which included a 50cm wide source margin around the 8 acre (181m x 181m) field in order to investigate the potential impact of high flux density in the margin. Four periods from Ajwa and Sullivan (2012) were studied using various ISCST3 runs and assumptions. This study found that

1. When the Gao et al.(2013) flux densities were used for the tarp and margin, measured monitor concentrations were substantially overestimated in 3 of the 4 periods studied. At this time, it is not possible to conclusively determine if this overestimation is due to model bias or to a bias in the dynamic chamber flux measurement technique.
2. The average ratio of margin flux density to tarp flux density during the four studied periods was 43.8. When this ratio was built into the ISCST3 simulations, the percentage of monitor concentration due to margin sources ranged from 39% to 58%, with an average of 45%. Thus under the assumption of 43.8:1 flux ratio, the margins contributed nearly half to the monitor concentrations.
3. Estimated monitor concentrations based on tarp sources versus margin sources were highly correlated. In these four periods, neither tarp only, margin only, nor tarp plus margin based simulations provided any obvious advantage in explaining the monitored concentrations. These two flux sources are very entangled in ISCST3 simulations and it is not possible based only on ISCST3 modeling to reject either flux source.
4. Concentration estimates based on the flux densities reported in Ajwa and Sullivan (2012), which assumed only a tarp origin, compared to concentration estimates based on back-calculation embodying tarp and margin sources, yielded very similar results in 3 of 4 periods.

5. Under the assumption that margin fluxes are 43.8 times higher than the tarp fluxes, when calculations omit the margin fluxes for this 8 acre field, the resulting estimated tarp fluxes are estimated at about 60% higher than they would be if margin fluxes were taken into account.

The idea that flux near the edge of a relatively impermeable tarp may be much higher than flux on the adjacent tarp is an important conceptual understanding and in our considerations within the Department of Pesticide Regulation, should be kept in mind. However, as a practical matter, it does not appear to have great significance in terms of estimating monitor concentrations. Ignoring the margin flux density would is compensated for by increases in apparent tarp flux on the order of 60% and thus downwind concentration estimates would remain about the same, regardless of explicit margin modeling.

cc: Frank C. Spurlock, Ph.D.

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Tables

Table 1. Comparison of initial back calculation results between original analysis and analysis using modified Field 1 coordinates

Period	Analysis	Slope	Intercept	r2	Significance
5	Modified Field	2.05	-0.99	9%	p=0.14
	Original	2.08	-1.35	10%	p=0.13
6	Modified Field	6.53	5.04	48%	p<.01
	Original	6.49	4.98	49%	p<.01
7	Modified Field	1.4	1.33	5%	p=0.21
	Original	1.4	1.34	5%	p=0.21
8	Modified Field	0.87	-0.92	83%	p<.001
	Original	0.87	-0.94	82%	p<.001

Table 2. Relationship between ISC estimated concentrations for modified 8 acre field (y) and Ajwa and Sullivans polygon defined field (x).

Period	slope	intercept	r2	p
5	0.99	-0.028	99.9	<.001
6	0.99	0.002	99.9	<.001
7	0.99	-0.001	99.9	<.001
8	0.99	-0.034	99.9	<.001

Offsite Monitoring Times			Flux Chamber Monitoring			Flux 1,3-d (ug/m2s)	
Period	Start	End	Time After Injection (h)	Corresponding Date/Time	Assigned Offsite Period	On tarp	In margin
5	6/5/11 7:00	6/5/11 12:00	23.5	6/5/11 7:00	5	1.04	72.35
6	6/5/11 13:00	6/5/11 18:00	27.5	6/5/11 11:00	5	4.47	232.57
7	6/5/11 19:00	6/6/11 0:00	31.5	6/5/11 15:00	6	7.29	311.76
8	6/6/11 1:00	6/6/11 6:00	35.5	6/5/11 19:00	7	5.59	93.19
			39.5	6/5/11 23:00	7	7.69	159.84
			43.5	6/6/11 3:00	8	3.16	183.92

Table 3. Correspondence between flux monitoring events (Gao et al. 2013) and offsite air monitoring events for 1,3-d for field 1 in Lost Hills Study. Zero hour for flux monitoring was 7:30A.M. June 4, 2011. Time after injection was midpoint of flux monitoring period.

		Gao et al. (2013) Flux ug/m2s	
Period	Ajwa and Sullivan flux ug/m2s	Tarp	Margin
5	1.89	2.76	152.46
6	6.49	7.29	311.76
7	1.78	6.64	126.51
8	0.87	3.16	183.92

Table 4. Comparison of flux estimated from back-calculation (Ajwa and Sullivan 2012) versus on tarp and off tarp (margin) flux measurements from Gao et al. (2013).

Table 5. Regression results of measured period concentrations regressed on ISCST3

		y=Measured			y=Margin flux based
Period	**Statistic**	**All**	**Tarp**	**Margin**	**x=Tarp flux based**
5	**p**	0.12	0.14	0.08	<.001
	r2	0.11	0.09	0.15	0.59
	Slope	0.40	0.74	0.68	0.83
	Intercept	-0.48	-0.99	2.25	-0.79
6	**p**	<.001	<.002	<.001	0.02
	r2	0.76	0.48	0.83	0.32
	Slope	0.75	0.90	1.81	0.38
	Intercept	0.59	5.04	0.74	3.77
7	**p**	0.35	0.20	0.35	0.01
	r2	0.00	0.05	0.00	0.33
	Slope	0.14	0.21	-0.78	0.12
	Intercept	1.95	1.33	7.53	1.72
8	**p**	<.001	<.001	<.002	<.001
	r2	0.79	0.83	0.46	0.52
	Slope	0.19	0.28	0.39	0.40
	Intercept	-1.54	-0.92	-0.63	4.75

concentration estimates based on margin and tarp flux, tarp only flux, and margin only flux (Gao et al. 2013). Last column is ISCT3 concentration estimates based on Gao et al. (2013) margin fluxes regressed on ISCT3 concentration estimates based on Gao et al. (2013) tarp fluxes. Statistically significant regressions shaded.

Period	p for regression	Slope	[mean msr]/[mean model]	Adjustment Factor
5	0.123	1.229	1.155	1.155
6	0.000	5.414	5.603	5.414
7	0.546	0.514	1.273	1.273
8	0.000	0.647	0.475	0.647

Table 6. Results of regressing measured monitor concentrations for each of periods 5-8 on ISCST3 modeled concentrations where the ratio of margin flux to tarp flux was fixed at 43.8. Assumed fluxes for the ISCST3 modeling were for tarp and margin sources: 1 ug/m2s and 43.8 ug/m2s, respectively. Periods 6 and 8 resulted in significant regressions. Periods 5 and 7 were not significant. Also calculated was the mean measured concentration divided by the mean modeled concentration. The adjustment factor was the regression slope when the regression was significant and the mean measured divided by mean modeled when the regression was not significant.

			95% Confidence Interval	
Period	Regression Significance	Slope	Lower	Upper
5	<.001	0.86	0.68	1.05
6	<.001	0.76	0.60	0.91
7	<.001	1.01	0.84	1.17
8	<.001	0.99	0.84	1.17

Table 7. Regression of monitor concentration estimates based on Ajwa and Sullivan (2012) on monitor concentration estimates where ISCST3 included both tarp and margin sources with margin: tarp flux ratio of 43.8:1.

Figures

Figure 1. Map of 8 acre field in Lost Hills Study showing original UTM coordinates (Ajwa and Sullivan 2012). Corner coordinates clockwise from the northeast corner are: 256589, 3926927; 256585, 3926746; 256404, 3926749; 256405, 3926930.000.

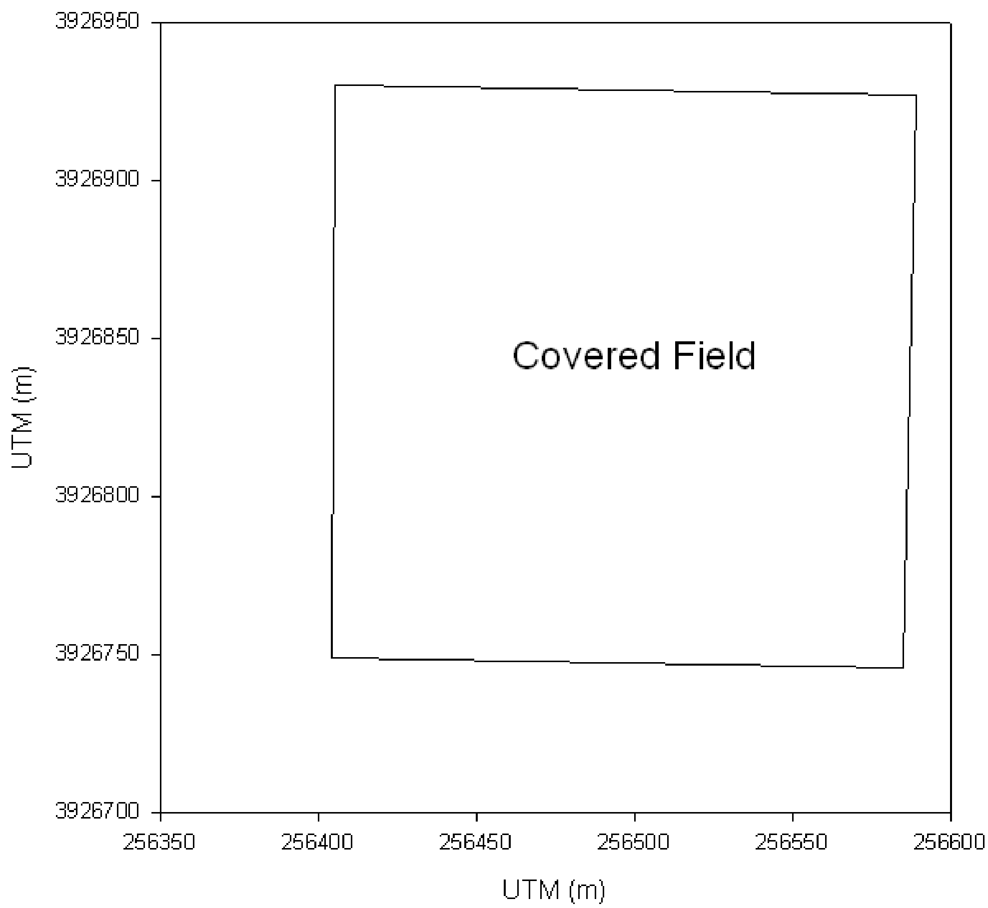


Figure 2. Northwest corner of idealized field representation. Shaded area is tarped field. Small rectangular areas around field are the margin sources (0.5m wide). Margin sources in graph correspond to sources M0036-M0042 in ISCST3 control file. The tarped field and margin sources represented two different source groups in the simulations.

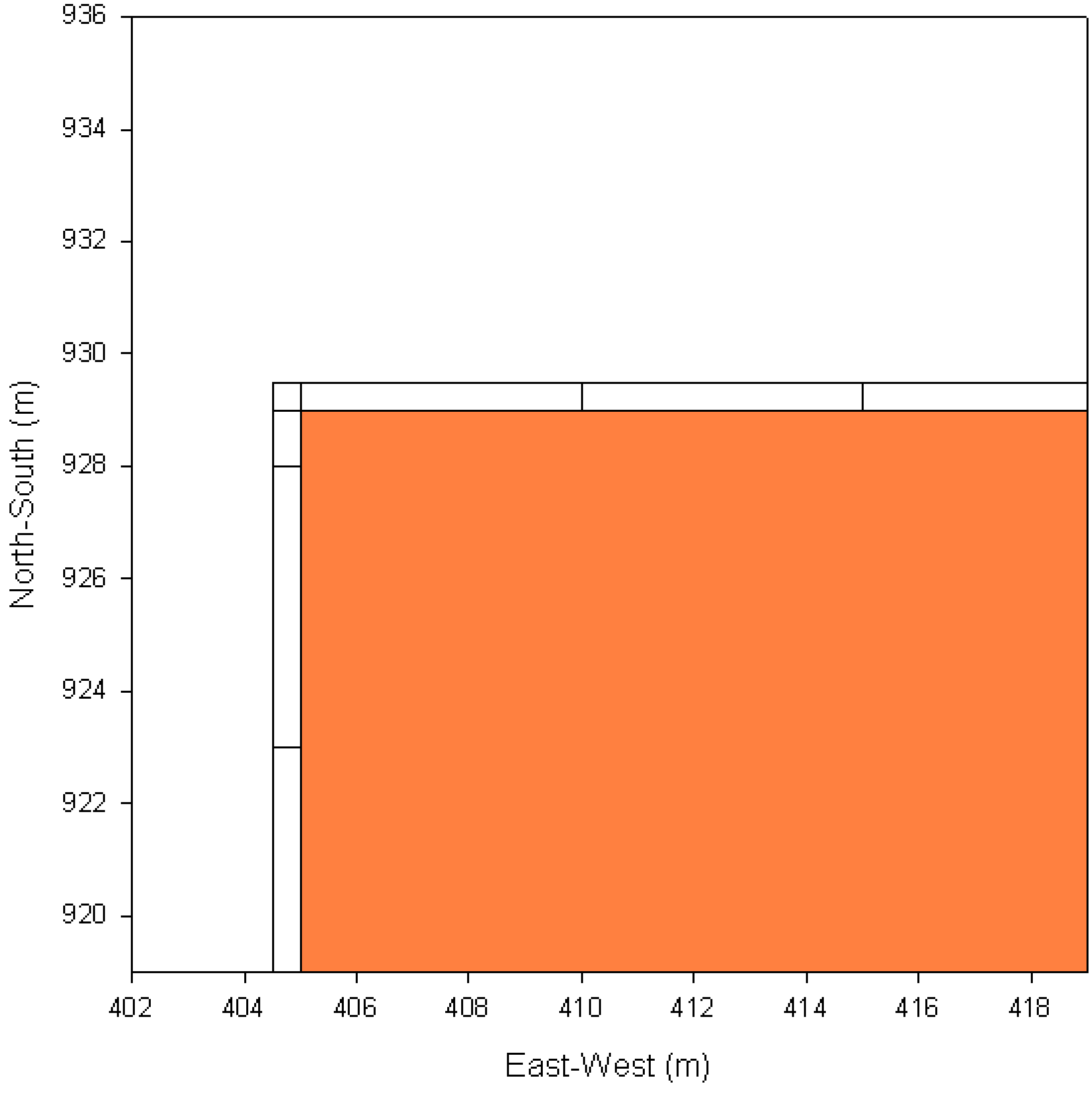
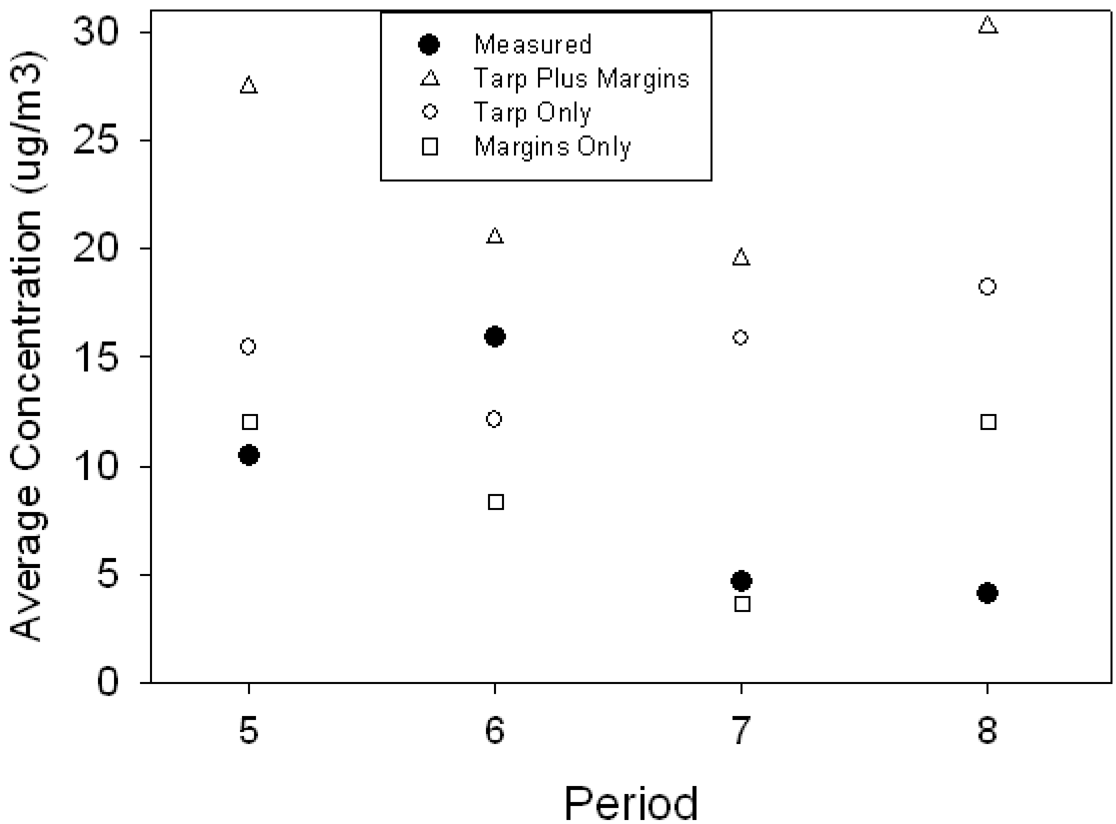


Figure 3. Period average concentration for measured concentrations, ISCST3 concentration estimates based on only tarp flux (excluding margins), only margin flux (excluding tarp), and the additive sum of margin and tarp flux where the fluxes were measured in Gao et al. (2013) (found in Table 3 of this memorandum).



Appendix. Example original and modified ISCST3 control files.

Original control file, Field 1, period 5, field represented as polygon

```
**
****************************************
**
** ISCST3 Input Produced by:
** AERMOD View Ver. 7.3.0
** Lakes Environmental Software Inc.
** Date: 12/27/2011
** File: C:\Lakes\AERMOD View\2011c\2011cf1\2011cf1.INP
**
****************************************
**
**
****************************************
** ISCST3 Control Pathway
****************************************
**
**
CO STARTING
   TITLEONE C:\Lakes\AERMOD View\2011c\2011cf1\2011cf1.isc
   MODELOPT DFAULT CONC  RURAL
   AVERTIME PERIOD
   POLLUTID 13D
   TERRHGTS ELEV
   FLAGPOLE 1.50
   RUNORNOT RUN
   ERRORFIL 2011cf1.err
CO FINISHED
**
****************************************
** ISCST3 Source Pathway
****************************************
**
**
SO STARTING
** Source Location **
** Source ID - Type - X Coord. - Y Coord. **
   LOCATION PAREA2       AREAPOLY   256589.000  3926927.000      145.000
** DESCRSRC Field 1 Area Source
** Source Parameters **
   SRCPARAM PAREA2         1.0E-06     0.000         4
   AREAVERT PAREA2       256589.000 3926927.000 256585.000 3926746.000
   AREAVERT PAREA2       256404.000 3926749.000 256405.000 3926930.000
   SRCGROUP ALL
SO FINISHED
**
****************************************
```

```
** ISCST3 Receptor Pathway
****************************************
**
**
RE STARTING
** DESCRREC "" ""
   DISCCART    256498.00   3926947.00  145.00    1.50
   DISCCART    256544.00   3926939.00  145.00    1.50
   DISCCART    256601.00   3926942.00  145.00    1.50
   DISCCART    256594.00   3926880.00  146.00    1.50
   DISCCART    256606.00   3926835.00  146.00    1.50
   DISCCART    256594.00   3926793.00  147.00    1.50
   DISCCART    256600.00   3926732.00  148.00    1.50
   DISCCART    256537.00   3926741.00  148.00    1.50
   DISCCART    256487.00   3926734.00  148.00    1.50
   DISCCART    256448.00   3926741.00  149.00    1.50
   DISCCART    256391.00   3926737.00  149.00    1.50
   DISCCART    256398.00   3926797.00  149.00    1.50
   DISCCART    256387.00   3926845.00  148.00    1.50
   DISCCART    256399.00   3926886.00  147.00    1.50
   DISCCART    256394.00   3926942.00  146.00    1.50
   DISCCART    256454.00   3926939.00  145.00    1.50
RE FINISHED
**
****************************************
** ISCST3 Meteorology Pathway
****************************************
**
**
ME STARTING
   INPUTFIL ..\..\..\AERMOD~1\2011c\met1isc.prn
   ANEMHGHT 10 METERS
   SURFDATA 99999 2011
   UAIRDATA 99999 2011
   STARTEND 2011 6 5 7 2011 6 5 12
ME FINISHED
**
****************************************
** ISCST3 Output Pathway
****************************************
**
**
OU STARTING
** Auto-Generated Plotfiles
   PLOTFILE PERIOD ALL 2011CF1.IS\PE00GALL.PLT
OU FINISHED
**
****************************************
** Project Parameters
****************************************
```

```
** PROJCTN  CoordinateSystemUTM
** DESCPTN  UTM: Universal Transverse Mercator
** DATUM    World Geodetic System 1984
** DTMRGN   Global Definition
** UNITS    m
** ZONE     11
** ZONEINX  0
**
```

Modified ISCST3 control file. Field 1, period 5, with field represented as perfect square with sides 181m x 181m. UTM coordinates shortened to 3 digit representation.

```
CO STARTING
   TITLEONE Gao flux, field, margin, field+margin PERIOD 5
   MODELOPT DFAULT CONC  RURAL
   AVERTIME 6 PERIOD
   POLLUTID 13D
**   TERRHGTS FLAT
   FLAGPOLE 1.50
   RUNORNOT RUN
   ERRORFIL margin.err
CO FINISHED
***************************************
** THE FIRST 1 BIG SOURCE IS THE IDEALIZED FIELD (SEE 'GET-IDEALIZED-
COORDINATES.XLSX')
** I HAVE MADE EVERYTHING AT ELEV OF ZERO AND
** I HAVE SUBTRACTED 256000 FROM THE X COORDINATES AND
** 3926000 FROM THE Y COORDINATES (ORIGINAL COORDINATES WERE UTM
** WITH sw CORNER AT ~256405,3926748
** [130125] for this one, set margins at 75 ug/m2s and kept field at same 1
ug/m2s
** am looking for regression with this fixed ratio.
***************************************
SO STARTING
SO LOCATION BIGMUTHA AREA 405. 748.
SO SRCPARAM BIGMUTHA 0.276E-5 0. 181.
**BEGIN MARGIN SOURCES
SO LOCATION M0001 AREA  404.50  747.50
SO LOCATION M0002 AREA  404.50  748.00
...
(margin source location records for M0003-M0152 omitted)
...
SO SRCPARAM M0001  0.152E-03 0.0   0.500   0.500
SO SRCPARAM M0002  0.152E-03 0.0   0.500   5.000

(margin srcparam records for M0003-M0152 omitted)


**END MARGIN SOURCES
SO SRCGROUP ACRE8 BIGMUTHA
SO SRCGROUP MARGIN M0000-M0152
SO SRCGROUP ALL
SO FINISHED
*****************************************
** RECEPTORS, NOTE X COORDS SUBTRACTED 256000
** Y COORDS, 3926000, AND ZEROED THE ELEVATION
*****************************************
```

```
RE STARTING
   DISCCART   498.00  947.00      1.5
   DISCCART   544.00  939.00      1.50
   DISCCART   601.00  942.00      1.50
   DISCCART   594.00  880.00      1.50
   DISCCART   606.00  835.00      1.50
   DISCCART   594.00  793.00      1.50
   DISCCART   600.00  732.00      1.50
   DISCCART   537.00  741.00      1.50
   DISCCART   487.00  734.00      1.50
   DISCCART   448.00  741.00      1.50
   DISCCART   391.00  737.00      1.50
   DISCCART   398.00  797.00      1.50
   DISCCART   387.00  845.00      1.50
   DISCCART   399.00  886.00      1.50
   DISCCART   394.00  942.00      1.50
   DISCCART   454.00  939.00      1.50
RE FINISHED

ME STARTING
   INPUTFIL met1isc.prn
   ANEMHGHT 10 METERS
   SURFDATA 99999 2011
   UAIRDATA 99999 2011
**   STARTEND 2011 6 4 19 2011 6 4 24
** PERIOD 5, 6 HOURS
   STARTEND 2011 6 5 7 2011 6 5 12
ME FINISHED
**
****************************************
** ISCST3 Output Pathway
****************************************
**
**
OU STARTING

   POSTFILE 6 ACRE8 PLOT mg03P5-8.PST
   POSTFILE 6 MARGIN PLOT mg03P5-mARG.PST
   POSTFILE 6 ALL PLOT mg03P5-all.PST

OU FINISHED
**
```

Source code listing for MARGINS01.FOR. Note word wrap causes some longer lines to be continued.

```
C     Last change:  BJ   16 Jan 2013    4:28 pm
        program margins01
ccccccccccccccccccccccccccc
c
c program margins01 takes as input
c lower left corner x and y coordinate and side length (assuming a square)
c
c and the width of the margin
c
c then calculates and formats a series of sources which will comprise a non-
overlapping margin
c around the field. for use with ISCST3
c
cnote: i tested this program with margins = 0.5, 1.0, and 2. and 1.27 and it
seemed to work.
c
ccccccccccccccccccccccccccc
        implicit none
        REAL LX,LY,S !LOWER LEFT X,Y COORDS FIELD, S IS SIDELENGTH
        REAL marg  !WIDTH OF MARGIN
        REAL MARGLEN  !10X WIDTH OF MARGIN
        INTEGER NUMBERWHOLES !NUMBER OF WHOLE LENGTH (marglen) MARGIN SOURCES
ALONG EACH SIDE
        REAL REMLEN !LENGTH OF LEFTOVER SOURCE
        !NOTE EACH MARGIN BEGINS WITH MARG X MARG SQUARE, THEN NUMBERWHOLES
RECTANGULAR
        !SOURCES MARG X 10*MARG IN DIMENSION, AND FINISHING WITH MARG X
REMLEN SOURCE
        !SO THAT THE MARGINS ARE COMPRISED OF 2 + NUMBERWHOLES SOURCES ALONG
EACH SIDE
        !FOR A TOTAL OF 4 X (2 + NUMBERWHOLES) SUBSOURCES
        !note that the first square is margxmarg and is started in a negative
position in relation to the side/direction
        !for example, the very first square on the west edge, has its SW
corner at x-marg,y-marg, then the next square
        !starts at SW corner of x-marg,y and is 10*marg high (so, marg x
10*marg, marg width in EW dir)
        CHARACTER*4 CC
        CHARACTER*70 LOCS(1000),SRCS(1000)
        INTEGER I, COUNT,K, NUMBSOURCES,NNN
        REAL FLUX,ELEV

        OPEN(UNIT=1,FILE='margins01.in',STATUS='old')
        OPEN(UNIT=2,FILE='MARGINS01.OUT',STATUS='UNKNOWN')
        READ(1,*)lx,ly,s
        READ(1,*)marg,FLUX,ELEV
```

```
        DO I=1,1000
          LOCS(I)(1:30)='123456789012345678901234567890'
          LOCS(I)(31:60)=LOCS(I)(1:30)
          LOCS(I)(61:70)=LOCS(I)(1:10)
          SRCS(I)=LOCS(I)
        END DO
        marglen=10*marg
        numberwholes=INT(s/marglen)
        remlen=s-numberwholes*marglen
        NUMBSOURCES=1+NUMBERWHOLES+1    !NUMBER OF SOURCES ALONG 1 EDGE PLUS
1 FOR MARGXMARG SOURCE
        NNN=NUMBSOURCES
        COUNT=0
        !west edge
        !CC(1:4)=CONVC(COUNT+1)
        K=COUNT+1

        CALL CONVC(K,CC)
        WRITE(locs(1),10)CC(1:4), lx-marg,ly-marg
10      FORMAT(' SO LOCATION M',A4,' AREA ',F7.2, 1X, F7.2)
        WRITE(SRCS(1),20)CC(1:4), FLUX, ELEV, MARG,MARG
20      FORMAT(' SO SRCPARAM M',A4,1X,E9.1,1X,F7.3,1X,F7.3,1X,F7.3)

        !NORTH EDGE
        K=COUNT+1+1*NNN
        CALL CONVC(K,CC)
        WRITE(LOCS(1+1*NNN),10)CC(1:4),LX-MARG,LY+S
        WRITE(SRCS(1+1*NNN),20)CC(1:4),FLUX,ELEV,MARG,MARG
        !EAST EDGE
        K=2*NNN+COUNT+1
        CALL CONVC(K,CC)
        WRITE(LOCS(1+2*NNN),10)CC(1:4),LX+S,LY+S
        WRITE(SRCS(1+2*NNN),20)CC(1:4),FLUX,ELEV,MARG,MARG
        !SOUTH EDGE
        K=3*NNN+COUNT+1
        CALL CONVC(K,CC)
        WRITE(LOCS(1+3*NNN),10)CC(1:4),LX+S,LY-MARG
        WRITE(SRCS(1+3*NNN),20)CC(1:4),FLUX,ELEV,MARG,MARG

       DO 30 I=1,NUMBERWHOLES
         !WEST EDGE
         COUNT=COUNT+1
         K=COUNT+1
         CALL CONVC(K,CC)
         WRITE(LOCS(COUNT+1),10)CC(1:4),LX-MARG,LY+(I-1)*MARGLEN
         WRITE(SRCS(COUNT+1),20)CC(1:4),FLUX,ELEV,MARG,MARGLEN
         !NORTH EDGE
         K=COUNT+1+1*NNN
         CALL CONVC(K,CC)
         WRITE(LOCS(COUNT+1+1*NNN),10)CC(1:4),LX+(I-1)*MARGLEN,LY+S
```

```
          WRITE(SRCS(COUNT+1+1*NNN),20)CC(1:4),FLUX,ELEV,MARGLEN,MARG
          !EAST EDGE
          K=COUNT+1+2*NNN
          CALL CONVC(K,CC)
          WRITE(LOCS(COUNT+1+2*NNN),10)CC(1:4),LX+S,LY+S-I*MARGLEN
          WRITE(SRCS(COUNT+1+2*NNN),20)CC(1:4),FLUX,ELEV,MARG,MARGLEN
          !SOUTH EDGE
          K=COUNT+1+3*NNN
          CALL CONVC(K,CC)
          WRITE(LOCS(COUNT+1+3*NNN),10)CC(1:4),LX+S-I*MARGLEN,LY-MARG
          WRITE(SRCS(COUNT+1+3*NNN),20)CC(1:4),FLUX,ELEV,MARGLEN,MARG
30       CONTINUE

         COUNT=COUNT+1
         !WEST EDGE
         K=COUNT+1
         CALL CONVC(K,CC)
         WRITE(LOCS(COUNT+1),10)CC(1:4),LX-MARG,LY+NUMBERWHOLES*MARGLEN
         WRITE(SRCS(COUNT+1),20)CC(1:4),FLUX,ELEV,MARG,REMLEN
         !NORTH EDGE
         K=COUNT+1+1*NNN
         CALL CONVC(K,CC)
         WRITE(LOCS(COUNT+1+1*NNN),10)CC(1:4),LX+NUMBERWHOLES*MARGLEN,
      *         LY+S
         WRITE(SRCS(COUNT+1+1*NNN),20)CC(1:4),FLUX,ELEV,REMLEN,MARG
         !EAST EDCGE
         K=COUNT+1+2*NNN
         CALL CONVC(K,CC)
         WRITE(LOCS(COUNT+1+2*NNN),10)
      *     CC(1:4),S+LX,LY
         WRITE(SRCS(COUNT+1+2*NNN),20)CC(1:4),FLUX,ELEV,MARG,REMLEN
         !SOUTH EDGE
         K=COUNT+1+3*NNN
         CALL CONVC(K,CC)
         WRITE(LOCS(COUNT+1+3*NNN),10)CC(1:4),LX,
      *    LY-MARG
         WRITE(SRCS(COUNT+1+3*NNN),20)CC(1:4),FLUX,ELEV,REMLEN,MARG

        DO I=1,4*NNN
          WRITE(2,50)LOCS(I)
50        FORMAT(1X,A70)
         END DO

        DO I=1,4*NNN
          WRITE(2,50)SRCS(I)
         END DO

        end program

         SUBROUTINE CONVC(N,CC)
```

```
      IMPLICIT NONE
      INTEGER N
      CHARACTER*4 CC
      INTEGER K

      CC(1:4)='XXXX'
      WRITE(CC,10)N
10    FORMAT(I4)

      DO K=1,4
       IF(CC(K:K).EQ.' ')CC(K:K)='0'
      END DO

      RETURN
      END
```

Example input file, MARGINS01.IN, for MARGINS01.FOR. Values are (first line) x,y (m) location for southwest corner of field, length of side of field (m), (second line) width of margin (m) around field, flux density (g/m2s) from margin, ELEV parameter (m) for ISCST3 control file.

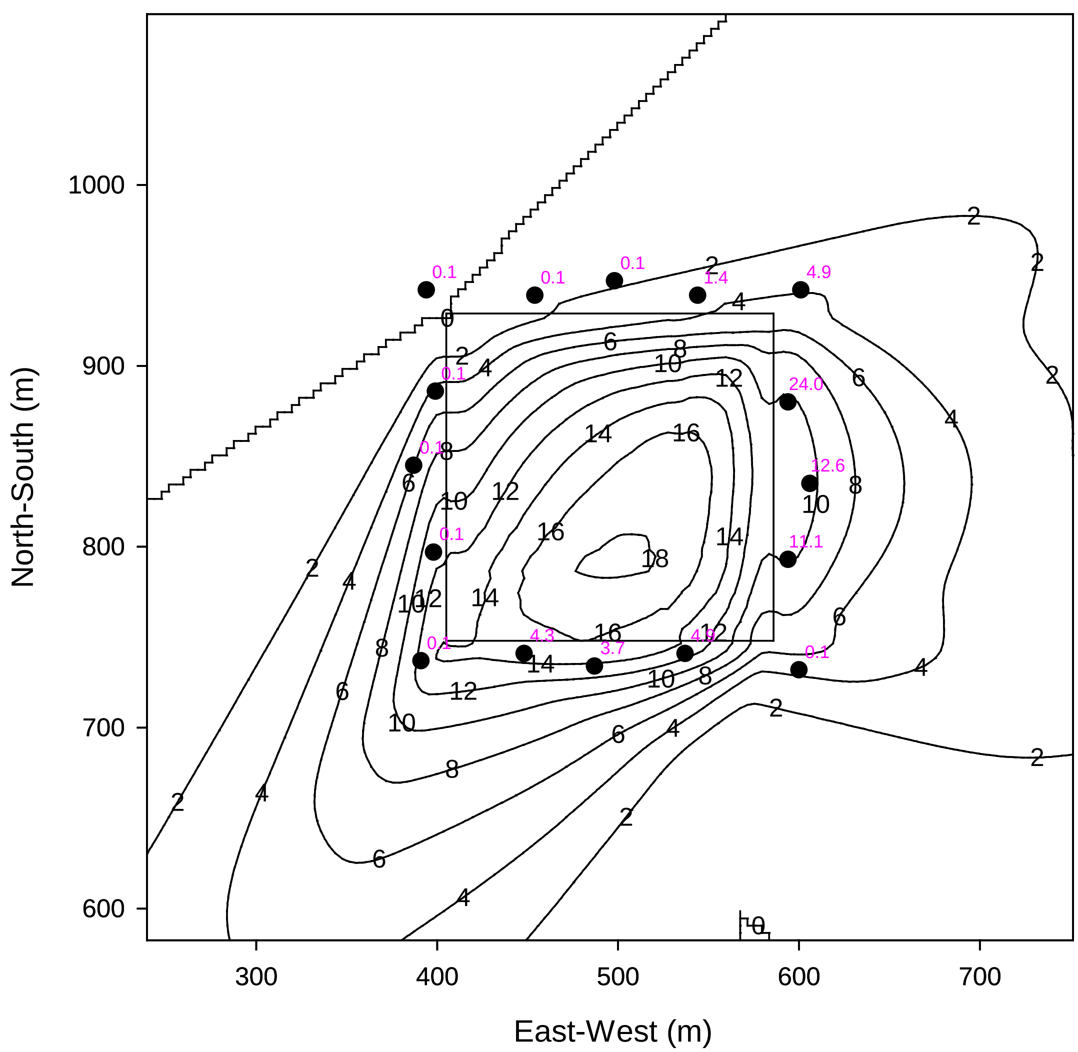
```
405. 748.  181.
.5  1.E-06   145.
```

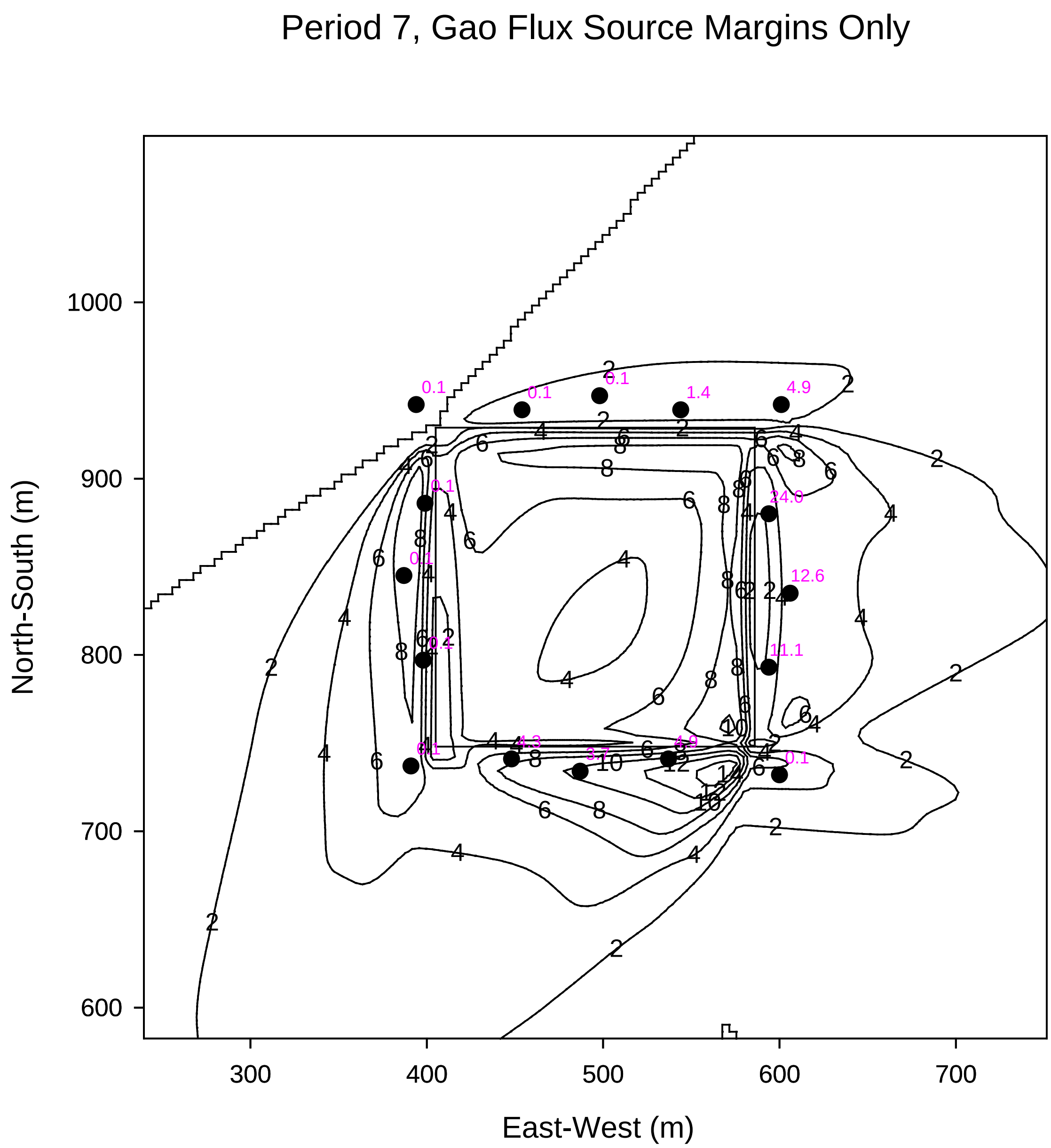
Portion of output file from MARGINS01.FOR.

```
  SO LOCATION M0001 AREA  404.50  747.50
  SO LOCATION M0002 AREA  404.50  748.00
  SO LOCATION M0003 AREA  404.50  753.00
  SO LOCATION M0004 AREA  404.50  758.00
  (M0005-M0152 omitted)
  SO SRCPARAM M0001   0.1E-05 145.000   0.500   0.500
  SO SRCPARAM M0002   0.1E-05 145.000   0.500   5.000
  SO SRCPARAM M0003   0.1E-05 145.000   0.500   5.000
  SO SRCPARAM M0004   0.1E-05 145.000   0.500   5.000
  (M0005-M0152 omitted)
```

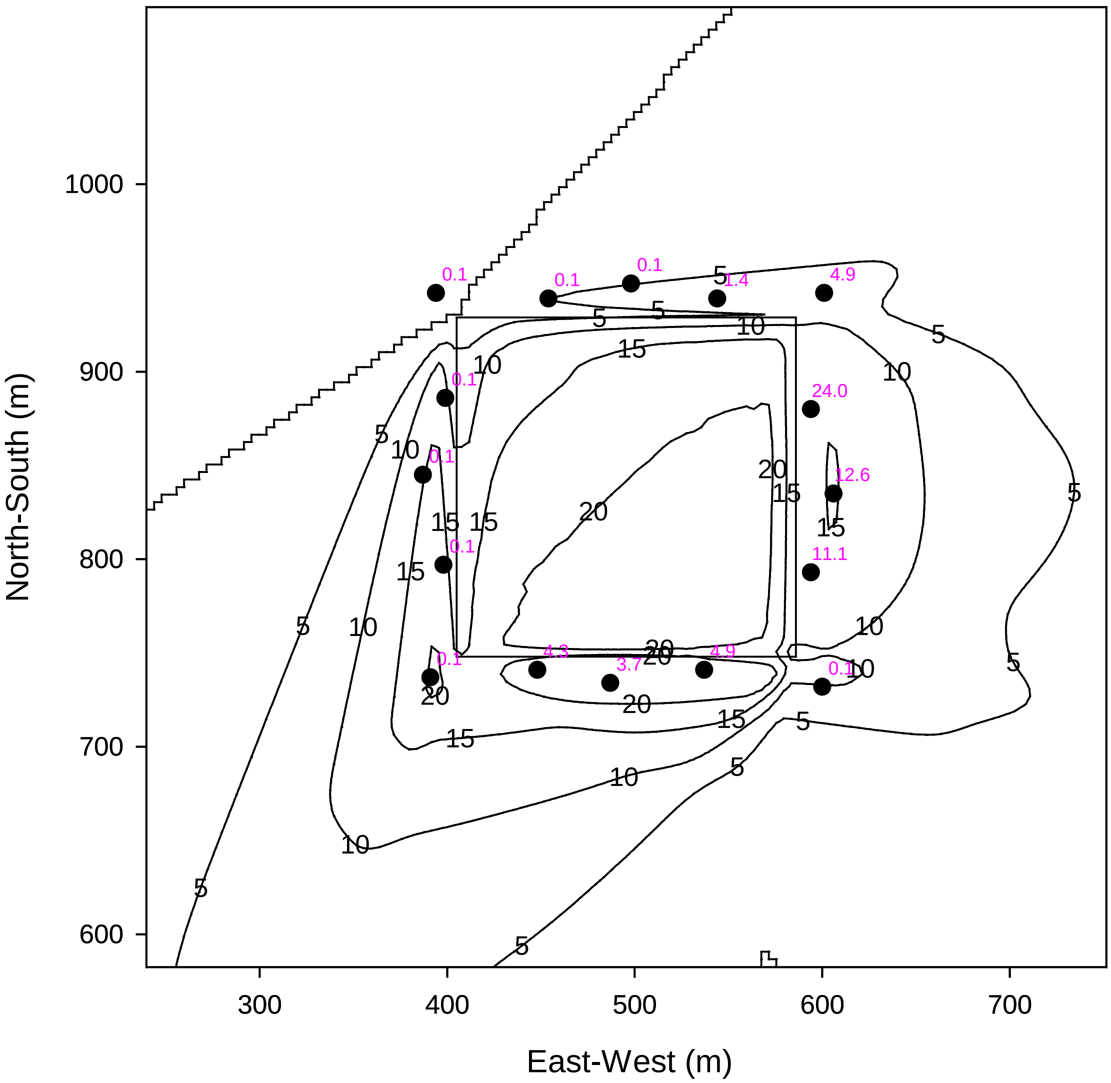
ISCST3-estimated concentration isopleths (ug/m3) for period 7 using flux density from Gao et al. (2013) with tarp flux source, margin flux source and tarp+margin flux source. Labeled points are receptor locations with measured concentrations (ug/m3) for that period.

Period 7, Gao Flux Source Tarp Only

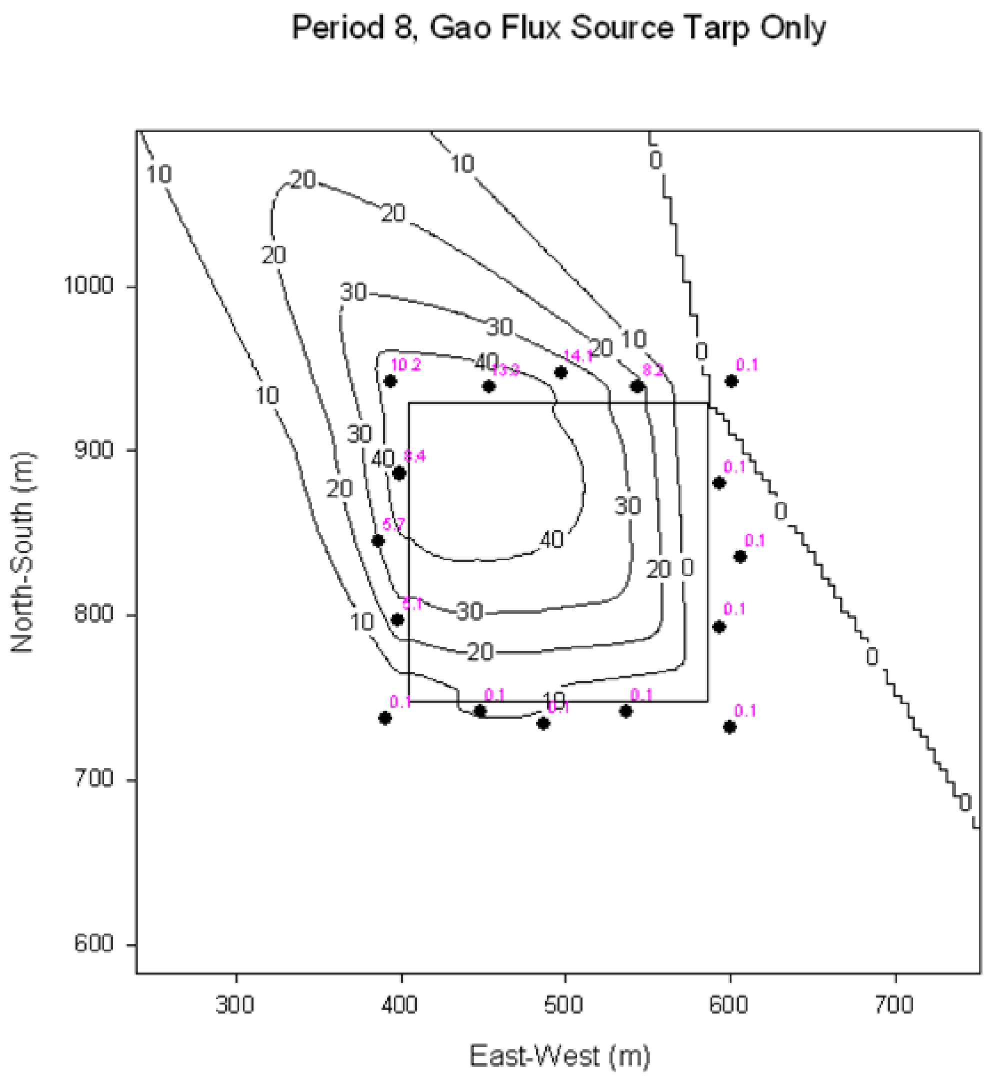


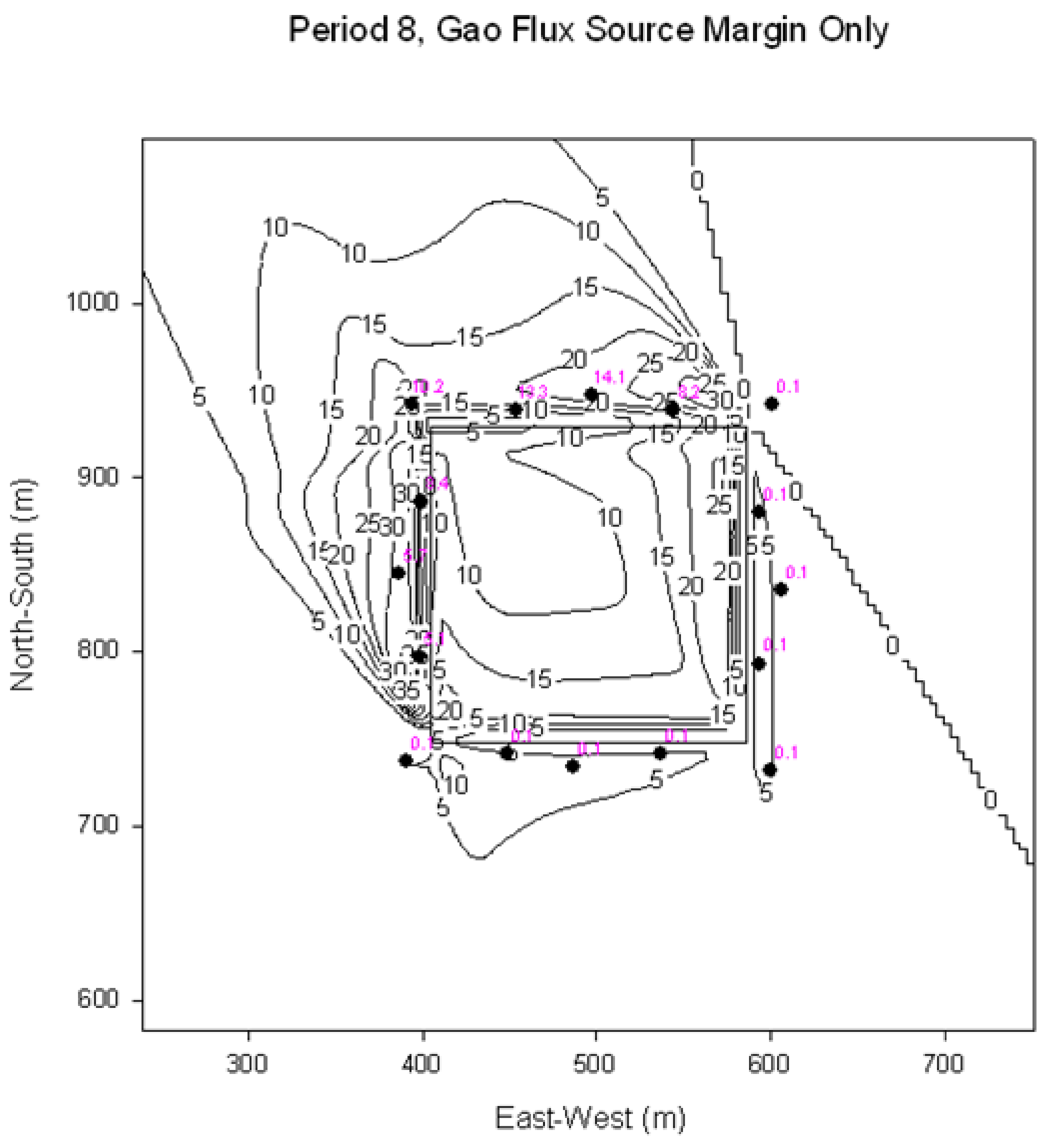

Period 7, Gao Flux Source Margins Only
North-South (m)
East-West (m)
1000
900
800
700
600
300
400
500
600
700
0.1
0.1
0.1
1.4
4.9
24.0
12.6
11.1
3.7
4.9
0.1

Period 7, Gao Flux Source Tarp+Margins

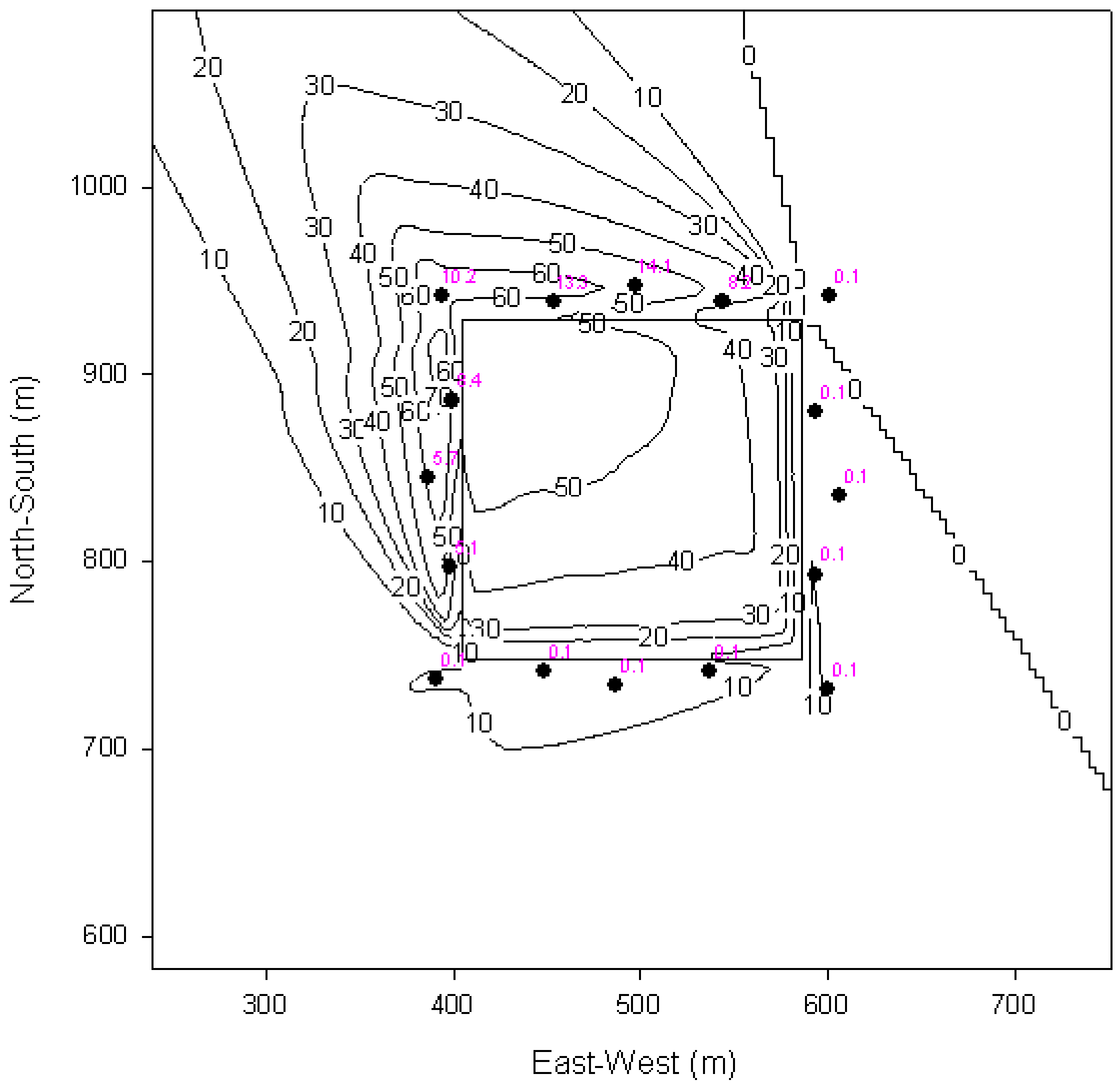


ISCST3-estimated concentration isopleths (ug/m3) for period 8 using flux density from Gao et al. (2013) with tarp flux source, margin flux source and tarp+margin flux source. Labeled points are receptor locations with measured concentrations (ug/m3) for that period.




Period 8, Gao Flux Source Margin Only
North-South (m)
East-West (m)
1000
900
800
700
600
300
400
500
600
700

Period 8, Gao Flux Source Tarp+Margin



Calculation Details for estimated flux through TIF based on laboratory measured permeability

	A	B	C	D	E
1	0.00004	cm/h	max possible MTC given measured value of 0.0000cm/h (Qian et al. 2011)		
2	3600	s/h	conversion factor		(I verified units for MTC in Qian et al. 2011, yes cm/h)
3	1.11111E-08	cm/s	max possible MTC in different units		
4	0.01	m/cm	conversion factor		
5	1.11111E-10	m/s	max possible MTCin different units in prep for concentration calculation		
6					
7	10	ug/cm3	approx max concentration of 1,3-d msrd beneath tarp in Lost Hills (Gao et al. 2013, Fig 1)		
8	1,000,000	cm3/m3	conversion factor		
9	10,000,000	ug/m3	approx max conc 13d different units		
10					
11	0.001111111	ug/m2s	flux density from product of MTC and max measured conc		
12					

Environmental Science & Technology — Article

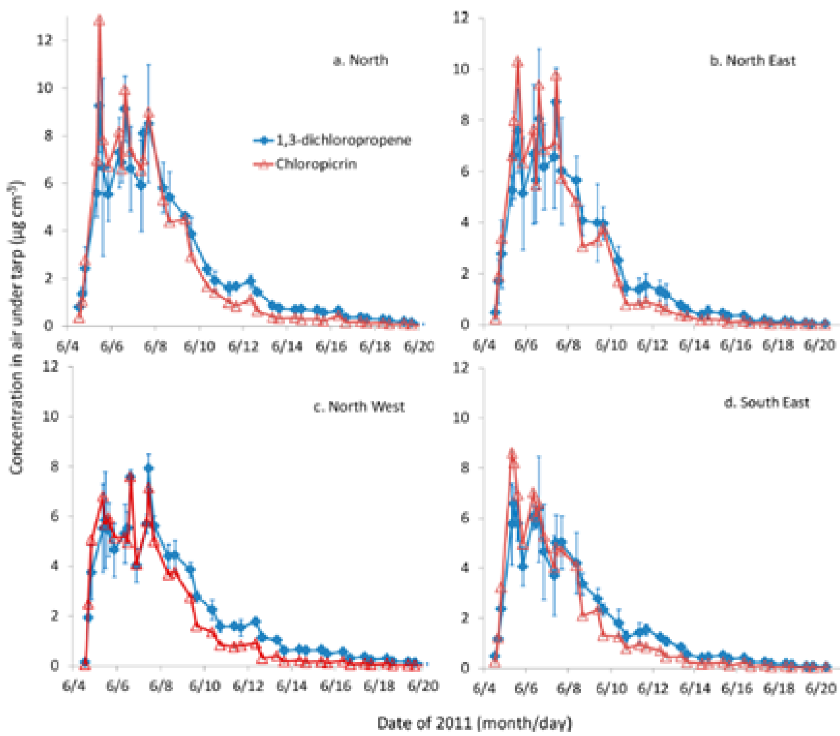


Figure 1. 1,3-Dichloropropene (1,3-D) and chloropicrin (CP) concentrations in air immediately under totally impermeable film (TIF) at four locations in a 3.3 ha fumigated field in 2011 in Lost Hills, CA. Pic-Clor 60 was broadcast applied via shank injections at 660 kg ha^{-1}. Error bars were standard deviation of three replicates for 1,3-D and error bars for CP were not plotted for readability.