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MEMORANDUM

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SUBJECT: ANALYSIS OF THE RELATIONSHIP BETWEEN PERCENTILES OF THE WHOLE FIELD BUFFER ZONE DISTRIBUTION AND THE MAXIMUM DIRECTION BUFFER ZONE DISTRIBUTION

Background

In 1992 the Department of Pesticide Regulation (DPR) first implemented the use of air dispersion modeling in the development of mitigation measures for bystander exposure to methyl bromide. The initial buffer zone development employed screening level modeling techniques, including standard weather conditions, square field geometry, and 24 hour time weighted average (TWA) flux (Johnson 1999, Johnson and Barry 2005, Segawa et al. 2000). The buffer zones developed were approximately 95% protective on an individual application basis (Johnson, 2001). This means that for any given application, the probability that the TWA concentration at the buffer zone distance would exceed a specified exposure threshold anywhere around the field perimeter was approximately 5%.

In recent years, with the development of probabilistic modeling packages (PERFUM [Reiss and Griffin, 2006]; FEMS [Sullivan et al., 2004]; SOFEA [Cryer, 2005]), distributions of buffer zones for various application scenarios have been produced using five year sets of meteorological data. As explained later, a buffer zone length at a particular percentile of the distribution insures coverage at a level of protection (protection probability) equal to that percentile. This technique of selecting a buffer zone length that corresponds to a desired protection probability from a distribution of lengths is now one of the most important air dispersion modeling based mitigation tools. However, two very different methods have been used to construct distributions of buffer zone lengths for specific use scenarios. Even though the resulting buffer zone distributions represent fundamentally different philosophies of risk mitigation and are not equivalent, the terminology used to describe the protection probability is the same. Consequently, there is substantial confusion over the meaning of "protection probability" and related concepts with these different methods.

The two methods for constructing a distribution of buffer zone lengths are known as the "whole field" method and the "maximum direction" method. The general modeling procedure used to determine the buffer zone distributions for either the maximum direction or whole field method starts with a given fumigant flux versus time function ("flux profile", e.g. Figure 1), which describes the course of emissions following an application. For a specific scenario the size of the field is fixed, as is the application rate. What varies from simulation to simulation is the meteorology used to calculate the downwind air concentrations. The downwind air concentrations are averaged over the appropriate exposure time (also called the threshold averaging period). The threshold averaging period and the threshold concentration (or reference concentration) is fumigant specific. For example, the DPR methyl bromide threshold averaging time is 24 hours and the DPR threshold concentration is 815 ug/m^3 as a 24-hr time TWA. In each period, the concentration isopleths generated by the model are compared to the concentration exposure threshold (for example, 815 ug/m^3 for methyl bromide). Buffer zones are determined by the distance from the field edge to where the threshold concentration occurs. Thus, the resulting buffer zone distributions reflect the variations in period-to-period meteorology.

For both methods discrete directions are represented as "spokes" emanating outward from the center of the field (e.g. Figure 2), and are defined by the discretization scheme used in the modeling procedure. However, for the maximum direction method, the comparison of concentrations on each spoke yields a single distance that is equal to the maximum distance at which the modeled TWA concentration is equal to the exposure threshold. This procedure is repeated over the length of the meteorology record and the distances are compiled to obtain a distribution. For example, for methyl bromide and using a 24 hour threshold averaging time, each day (24 hours) of simulation yields a single buffer zone estimate. In this case a 5 year simulation would provide approximately 365 x 5 = 1825 daily, maximum buffer zones which would be compiled to form a distribution. The number is approximate because meteorological data sets may be incomplete.

In contrast, the whole field method compiles distances in every direction around the field during each threshold averaging period for each simulation. The number of distances selected in each averaging period is equal to the number of spokes, and each selected distance is equal to the distance along the spoke where the modeled TWA concentration equaled the exposure threshold. Then, similar to the maximum direction method, the procedure is repeated over the length of the meteorology record to generate the whole field buffer zone distribution. For example, a single threshold averaging period simulation for methyl bromide (24-hour) would yield 200 buffer zone estimates (if the field had 200 spokes). The maximum of the 200 buffer zone estimates is the maximum direction buffer zone distance for that day. The remaining 199 estimates will generally be less than the maximum. In the whole field method, all 200 daily buffer zone estimates are compiled from each day to form the distribution. This results in approximately
365 x 5 x 200 = 365,000 estimates.

In developing fumigant buffer zones by both the screening approach and the probabilistic approach, DPR has controlled protection probabilities at the individual application level (Segawa et al. 2000, Johnson, 2001, Barry, 2006). To do this, for each threshold averaging period the single point farthest away from an application where the threshold concentration occurs determines the buffer zone for each realization of an application scenario. For example, over the long term, a buffer zone selected to be “95%” protective for a 24 hour TWA threshold will be long enough to capture the threshold air concentration everywhere around the perimeter of the field for 95% of all applications. Thus, on average over thousands of realizations, for every 100 applications, the buffer zone will be large enough for 95 of those applications–the buffer zone achieves the protection goal. However, 5 of those 100 applications will show air concentrations at the buffer zone that exceed the threshold air concentration. Thus, the buffer zone fails to achieve the protection goal at some locations around the perimeter of the field. This “maximum direction buffer zone” method (Reiss and Griffin, 2006) of constructing the protection probability controls individual application risk. Barry and Johnson (2005) previously verified the PERFUM maximum direction buffer zone protection probabilities.

While the whole field approach (Reiss and Griffin, 2006) employs the same general modeling procedure as the maximum direction method, the whole field buffer zone distributions are constructed using distances to the threshold air concentration in every direction around the field during each averaging period. Thus, the whole field approach includes in its distributions distances which are predominantly upwind and, therefore, small. The whole field buffer zone percentiles are equal to the probability that the TWA concentration is less than or equal to the threshold at any random location along the edge of the buffer zone of a random application. The whole field buffer zone percentiles do not correspond to a specified level of protection at the individual application level. Therefore it is important to determine the relationship between the maximum direction and whole field approaches in terms of the per application failure rate.

If risk managers are to make fully informed decisions, the method with which the protection probability is constructed must be completely transparent and well understood. The objective of this memorandum is four fold: (1) to describe procedures and assumptions used to derive the PERFUM whole field and maximum direction buffer zone distributions, (2) to provide a transparent comparison of the whole field method protection probabilities to the equivalent maximum direction protection probabilities using actual model fumigant datasets, (3) to verify in a specific scenario PERFUM2 calculations, and (4) to estimate in a specific scenario the distribution of perimeter fractions amongst days where the buffer zone was not protective. Our intent is to provide risk managers and stakeholders with a technical analysis that assists the process of risk mitigation.

Methods

Two types of data were used in this analysis to characterize the relationship between the maximum direction protection probability and the whole field protection probability: (1) Data collected from PERFUM outputs for modeling conducted by the U.S. Environmental Protection Agency (EPA) and (2) data calculated using PERFUM code modified to provide air concentration and buffer zone outputs not available from the distributed model.

Data collected from the USEPA PERFUM modeling outputs

PERFUM modeling results were obtained from U.S. EPA as part of the materials DPR staff reviewed related to U.S. EPA fumigant risk assessments. For the present analysis, PERFUM outputs for various soil applications of methyl bromide, chloropicrin and metam sodium under various meteorological data sets were used to assemble a database containing the 99th percentile (99%) whole field buffer zone length and its equivalent maximum direction percentile (rounded to the nearest 1%). The equivalent maximum direction percentile is the percentile of the maximum direction buffer zone distribution that corresponds to a buffer zone equal to the 99% whole field buffer zone length, and is numerically equal to the individual application level maximum direction protection probability. This procedure is illustrated graphically in Appendix F. The five meteorological data sets (locations) were: (1) Ventura, California, (2) Bakersfield, California, (3) Tallahassee, Florida, (4) Yakima, Washington, and (5) Flint, Michigan. Simulations were conducted at maximum application rates and differing application methods, specific to each fumigant. Comparisons between the 99% whole field buffer zones and the equivalent maximum direction percentiles are presented graphically and statistical summaries are included.

The objective was to characterize the relationship between the 99% whole field buffer zone length and its equivalent maximum direction buffer zone length distribution percentile over field sizes of 5, 20, and 40 acres. However, a significant limitation is the PERFUM 1440m upper limit on buffer zone length output. Because it is not possible to estimate percentiles for buffer zone lengths generated by PERFUM which are at or exceed 1440m, it was necessary to exclude from this analysis those fumigant application method, rate and size combinations that would produce large buffer zones which exceeded 1440m. Therefore, this analysis cannot fully characterize the relationship between the 99% whole field buffer zone distributions and the maximum direction buffer zone distributions.

PERFUM Code Modification

Modifications were made to the PERFUM2 source code in order to externally record internally generated values of interest (more on the modifications below). Using this modified code, 2 pesticide application situations were studied: 5 acre with fine grid and 20 acres with fine grid. The application scenario was shallow shank injection, tarped methyl bromide application using the maximum application rate of 430 lbs/acre. The flux profile is shown in Figure 1. While two 24-hour periods were included in the flux profile, the analysis focused on the first 24-hour period, which was the highest flux period. A listing of the PERFUM2 input file for 20 acres is shown in Appendix A. Ventura meteorology was used, though one day was removed due to a string of 24 hours of calms.

The PERFUM2.FOR source code was modified to print out daily concentrations ordered by both spoke/ring and spoke-specific buffer information. The modifications were exclusively in the subroutine “DAYCALC”, which is contained in the PERFUM2.FOR file. The modifications are described more fully in Appendix B and a FORTRAN source code listing showing the modifications is presented in Appendix C. Briefly, code was inserted to open files and write out internal values. The code modifications did not change the logic or calculations of the program.

These modifications in the subroutine DAYCALC provided output which enabled (1) verification of the individual concentrations averages generated by PERFUM2, (2) analysis of the number of spokes each day where the reference concentration was exceeded along that spoke at the buffer zone distance, (3) verification of the 99% whole field buffer distance, and (4) further analysis of the fraction of the perimeter at the buffer zone distance where the health reference concentration would be exceeded. For (1) a single day was chosen, an independent ISCST3 control file was created and the discrete receptor concentrations from the single-day independent run were compared to the corresponding concentrations from PERFUM2 as found in CONCEN.OUT. For (2) the 99% whole-field buffer zone was compared to each spoke-specific buffer zone each day. The daily spoke exceedance information was used to estimate a daily fraction of the buffer perimeter where the reference concentration was exceeded. These daily lengths were compiled into a distribution. For (3) the individual spoke length “buffers” (distance to reach the reference concentration) were aggregated into a distribution and distributional points were compared to the PERFUM2 distribution points. For (4) an additional program was written to analyze output from the modified PERFUM2 to calculate a fraction of the perimeter where concentrations exceeded the reference concentration.

For days on which concentrations along the buffer zone exceeded the reference concentration, we calculated the fraction of the perimeter that exceeded the reference concentration with two methods: by a simple count of exceedance spokes divided by total spokes and by an edge/corner spoke perimeter calculation that adjusted for the different arc-length represented by the edge versus corner spokes. There was no substantive difference in these results, so the perimeter calculations based on the more accurate arc-length are presented. In this discussion, the edge/corner spoke method is the same as the arc-length method. Appendix D lists a FORTRAN utility which estimated the fraction of perimeter at the buffer zone distance where the threshold concentration was exceeded and Appendix E presents results comparing the two methods for computing the perimeter distances where the threshold concentration was exceeded.

Results

Data collected from the USEPA PERFUM modeling outputs

Figures 3 through 5 show the change in the equivalent maximum direction buffer zone distribution percentile with the 99% whole field buffer zone length. The three figures are on the same scale to facilitate cross comparison. For methyl bromide (Figure 3) the equivalent maximum direction percentiles are clustered between about 85% and 90%. For metam sodium (Figure 4) and chloropicrin (Figure 5), the equivalent maximum direction percentiles show a greater range, from about 95% to 63%. There are several factors potentially contributing to differences observed between fumigants. The most significant factor may be the averaging time of the health threshold. The methyl bromide averaging time is 24 hours, the metam sodium averaging time is 8 hours, and the chloropicrin averaging time is 4 hours. It should be noted that the health threshold air concentration for metam sodium applications is actually for methyl isothiocyanate, which is a breakdown product of metam sodium and the contaminant of concern. An additional factor is that the 4-hr and 8-hr TWA whole field buffer zones with the lowest maximum direction buffer equivalent percentile occurred at night. Thus, shorter threshold averaging time coupled with a flux profile that caused the whole field buffer zone size to be driven by nighttime averaging periods was associated with the lowest maximum buffer zone equivalent percentiles.

Figure 6 summarizes the relationship between the 99% whole field buffer zone length and the equivalent percentile in the maximum direction buffer zone distributions for application methods used to apply the three fumigants. Figure 6 shows the distribution of maximum direction buffer zone percentiles with the median value labeled for each application scenario. The width of the box plots illustrates the variability for each application method in the equivalent maximum direction distribution percentiles. The methyl bromide 99% whole field buffer zones are the least variable with consistent median maximum direction buffer zone percentiles of 86 to 88. Thus, under the use scenarios characterized in this analysis on average about 12% to 14% of methyl bromide applications with a 99% whole field buffer zone will have a buffer zone failure somewhere along the whole field buffer zone perimeter. Figure 6 clearly shows variable performance of the 99% whole field buffer zones for metam sodium and chloropicrin. The median equivalent maximum direction percentiles vary between a high of the 92.5 and a low of 71. In addition to the large spread in the median equivalent maximum direction percentile for metam sodium and chloropicrin application methods, the variability within any particular application method is also quite different. For example, the metam sodium intermittent sprinkler and intermittent shank methods show very little variation and median equivalent maximum direction buffer zone percentiles of 91% and 92.5% respectively. In contrast, chloropicrin untarped broadcast and untarped bed methods show highly variable equivalent maximum direction buffer zone percentiles with median percentiles of 71% and 74.5%, respectively.

PERFUM Code Modification

Verifications. The single day verification showed complete agreement between the PERFUM2-generated concentrations and those from an independent ISCST3 run. The independently assembled distributions of whole-field buffer zone lengths yielded a 99% whole field buffer zone which agreed with the PERFUM2 99% whole field buffer zone for the 5 acre and 20 acre find grid scenarios. There was a minor difference in that PERFUM2 appears to round the estimated buffer zones to the nearest 5m. These verifications provide additional confidence in the PERFUM2 calculations.

Distributions of exceedance perimeter lengths. From the total 1794 days simulated, the 99% whole field buffer was not protective at some point along the perimeter of the buffer zone distance from the field on 271 days and 230 days for the 5 acre and 20 acre fields, respectively. Thus the 99% whole field buffer corresponded to an 85%-tile (=100*(1794-271)/1794) and 87%-tile (=100*(1794-230)/1794) maximum direction buffer for the 5 and 20 acre scenarios, respectively. These independently derived calculations were consistent with the results in Figure 6 for methyl bromide method 1.

Amongst the days where exceedances occurred, Figures 7 and 8 provide distributions for the fraction of the buffer zone perimeter based on the arc-length method which exceeded the reference concentration. The two methods for calculating the fraction yielded somewhat different histograms, but the general limits and shapes were similar (details in Appendix E). In both cases perimeter fractions ranged from 0.01 to about 0.15. In part, the differences between the 2 methods resulted from the different number of edge versus corner spokes between 5 acre and 20 acres fields and the relatively different arc lengths represented by the 5 acre and 20 acre cases.

The histograms in Figures 7 and 8 provide some indication of the distribution of fractions of perimeters which are exceeded, when there is an exceedance somewhere along the buffer zone perimeter. Figures 9 and 10 provide the same data expressed as cumulative distributions of perimeter exceedance fractions and can be utilized more quantitatively to calculate probabilities.

Thus, for example, for the 20 acre field, amongst days when there is an exceedance, the probability is about 50% that the length along the buffer zone distance perimeter will be greater than about 7% of the perimeter, using the arc-length perimeter calculation method (Figure 10).

Given that the 20 acre buffer perimeter for a 99% whole field buffer of 200m is 2,395m, there will be a 50% probability that the distance of exceedance along the buffer perimeter is greater than 168m.

Discussion

The 99% whole field buffer zones show median equivalent maximum direction buffer zone percentile levels of between 71% and 92.5% (Figure 6). Thus, the individual application 99% whole field buffer zone median failure rate is between 7.5% and 29% of applications. The highest failure rate of 37% was for chloropicrin broadcast untarp application method at Tallahassee, Florida.

The failure rate appears to be related to the averaging time of the health threshold. Shorter averaging times show higher individual application failure rates. Thus, the per application buffer zone failure rate determined using the 99% whole field method (ostensibly a 1% failure rate) results in maximum direction median failure rates of between 7.5% and 29% of applications. These results are for application scenarios where both the whole field and the maximum direction buffer zones are less than or equal to 1440m. Performance of large (>1440m) 99% whole field buffer zones is unknown.

For the 20 acre methyl bromide application example that we analyzed, when there is a failure, the data extracted from PERFUM indicates that the perimeter distances along which the health reference level is exceeded can be larger than the length of a football field. We would expect that varying field size, flux profile, or exposure period would influence the shape of the distributions in Figures 7-10 and hence, influence the size of the expected perimeter lengths which would be expected to experience concentrations higher than the reference level.

While the “whole field” method (Reiss and Griffin, 2006) has the stated objective of characterizing “whole population” risk, that method does not incorporate a numeric or spatial distribution of potentially exposed bystander populations. Consequently the whole field method does not explicitly incorporate the probability that bystanders are located on or near the buffer zone perimeter. The implicit assumption is that the probability is low and uniformly distributed around the field (Freeman, 2004). However, analysis of DPR soil application methyl bromide worksite plans (Barry, 2005) shows approximately 20% of applications have at least one sensitive site (e.g., residences, high schools) within 50ft of the buffer zone. The majority of applications showed between 1 and 10 sensitive sites and fewer showed between 10 and 50 or more (e.g. larger residential developments).

Summary

- The relationship between maximum direction and whole field buffer zone procedures was studied.

- The 99% whole field buffer zones corresponded to median equivalent maximum direction percentiles of 71% to 92.5%. This corresponds to a median individual application buffer zone failure rate of between 7.5% and 29%. The highest individual application buffer zone failure rate was 37% for the chloropicrin broadcast untarp application method at Tallahassee, Florida.

- Metam sodium and chloropicrin exhibited a wider range of equivalent percentiles than methyl bromide due to the shorter exposure threshold periods.

- Additional verification of PERFUM2 calculations was satisfactory.

- For a 20 acre methyl bromide shallow tarped scenario, amongst days where a 99% whole field buffer was exceeded, there was a 50% probability that the length of the perimeter that was exceeded would be greater than 168m.

- The whole field method does not take into account specific population locations and in California, residential development can be found next to approximately 20% of treated fields at the buffer zone distance.

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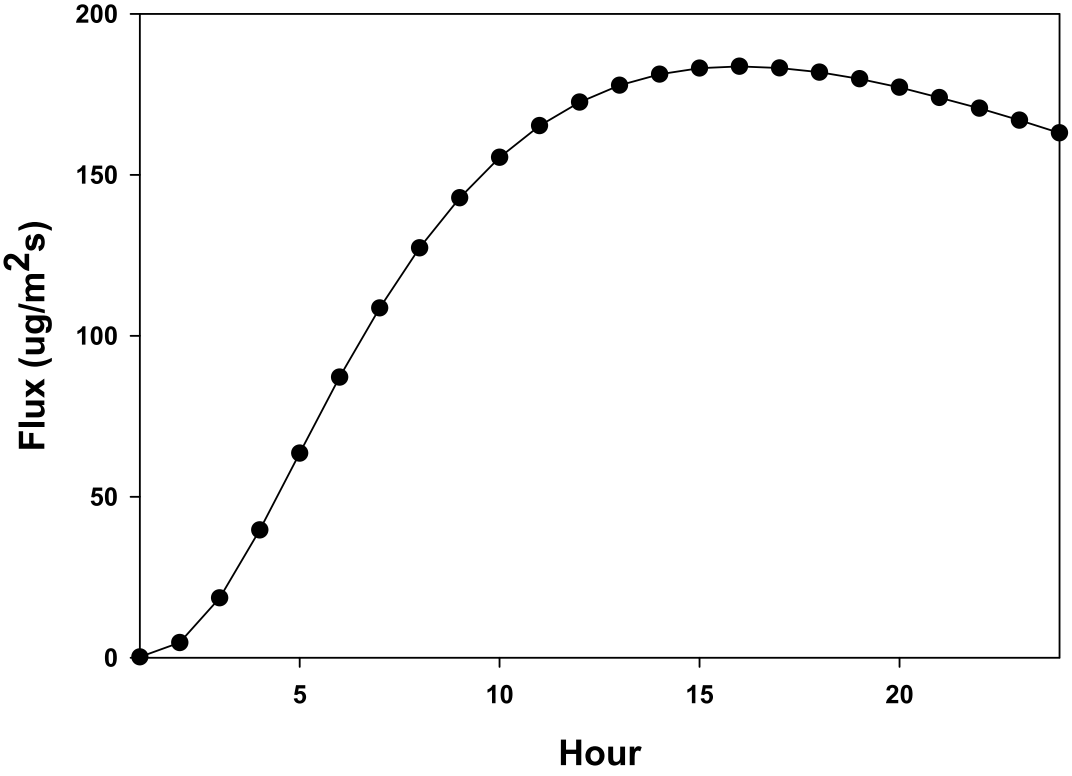


Figure 1. Flux profile for methyl bromide for first 24 hours.

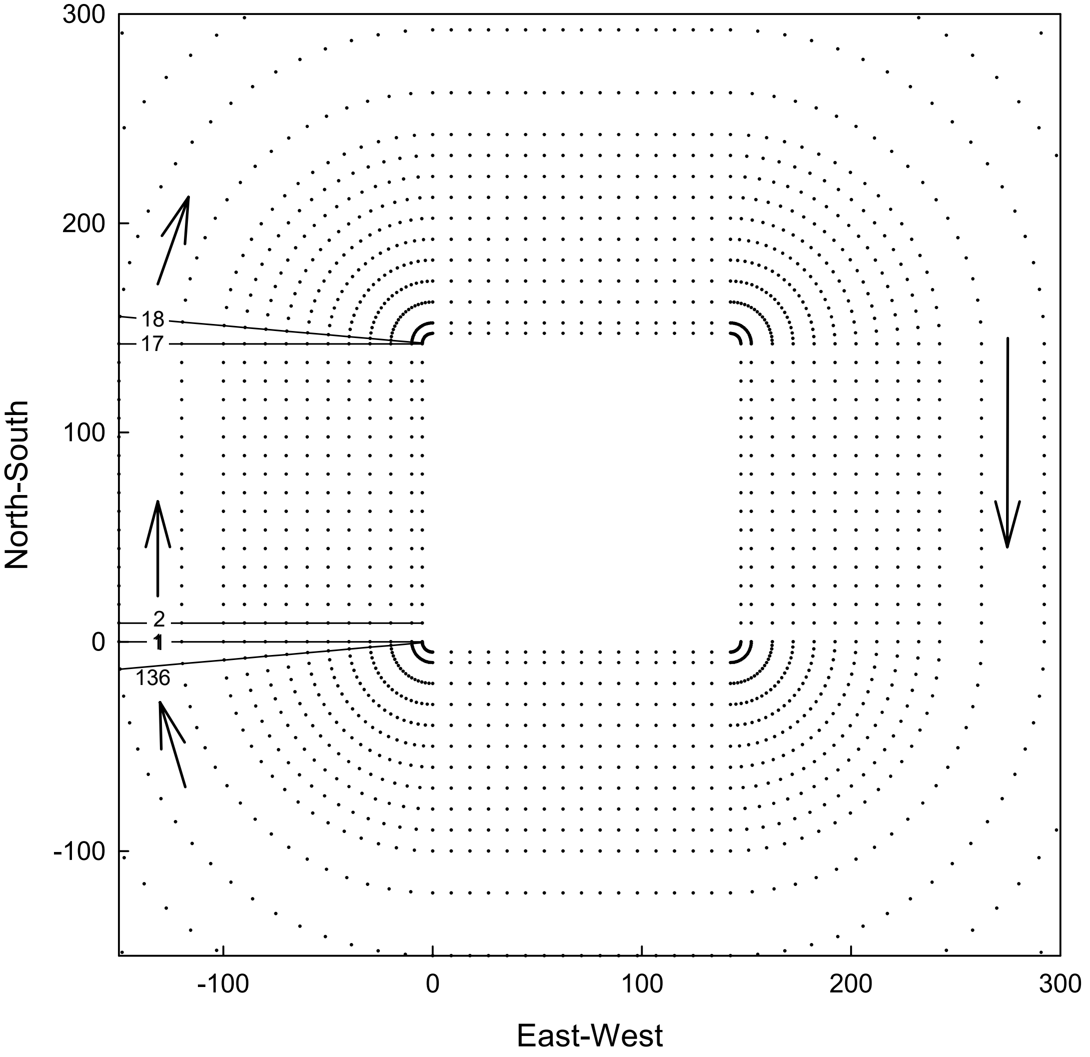


Figure 2. Spoke numbering scheme for 5 acre, square plot, fine grid. First spoke begins at southwest corner of field, extending due west. Subsequent spokes originate from the edge moving clockwise. There are 17 spokes along each straight edge and 17 spokes radiating from each corner, for a total of 136 spokes. Lines are drawn for illustration purposes for spokes 1,2,17,18 and 136.

Figure 3. Relationship between the methyl bromide 99% whole field buffer zone length (m) and the equivalent maximum direction buffer zone percentile. Equivalent maximum direction percentile = individual application level protection probability = (1 – individual application buffer zone failure rate).

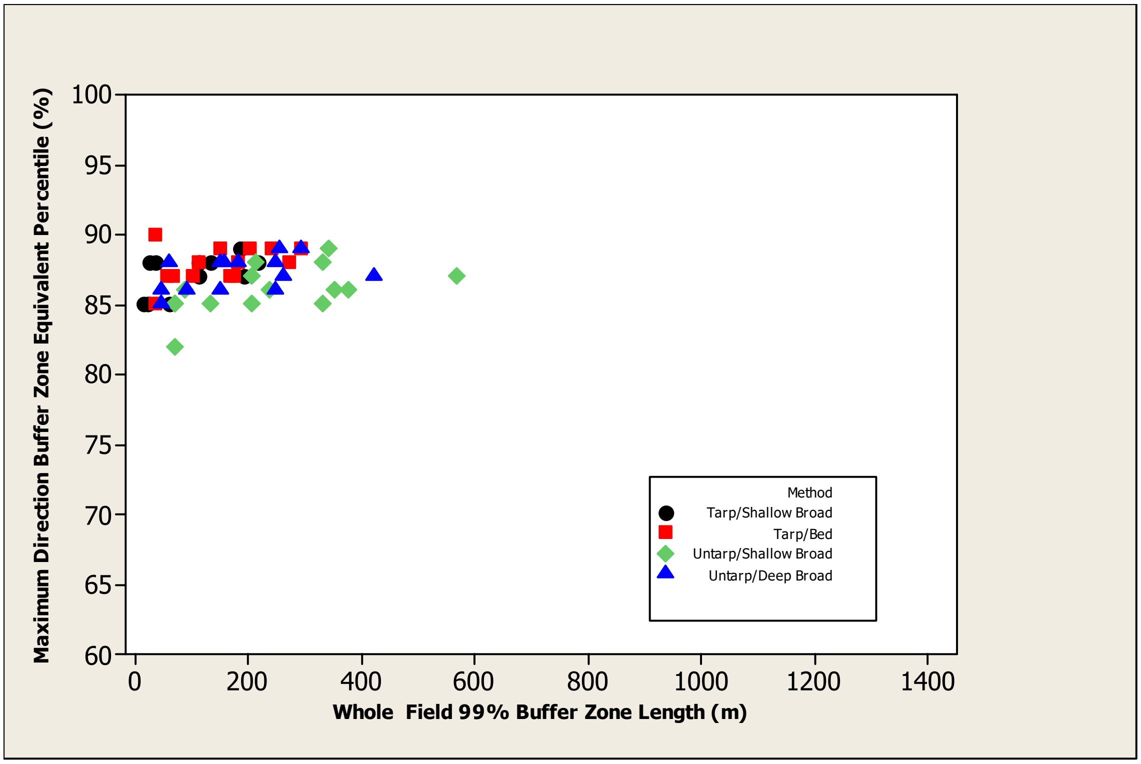


Figure 4. Relationship between the metam sodium 99% whole field buffer zone length (m) and the equivalent maximum direction buffer zone percentile. Equivalent maximum direction percentile = individual application level protection probability = (1 – individual application buffer zone failure rate).

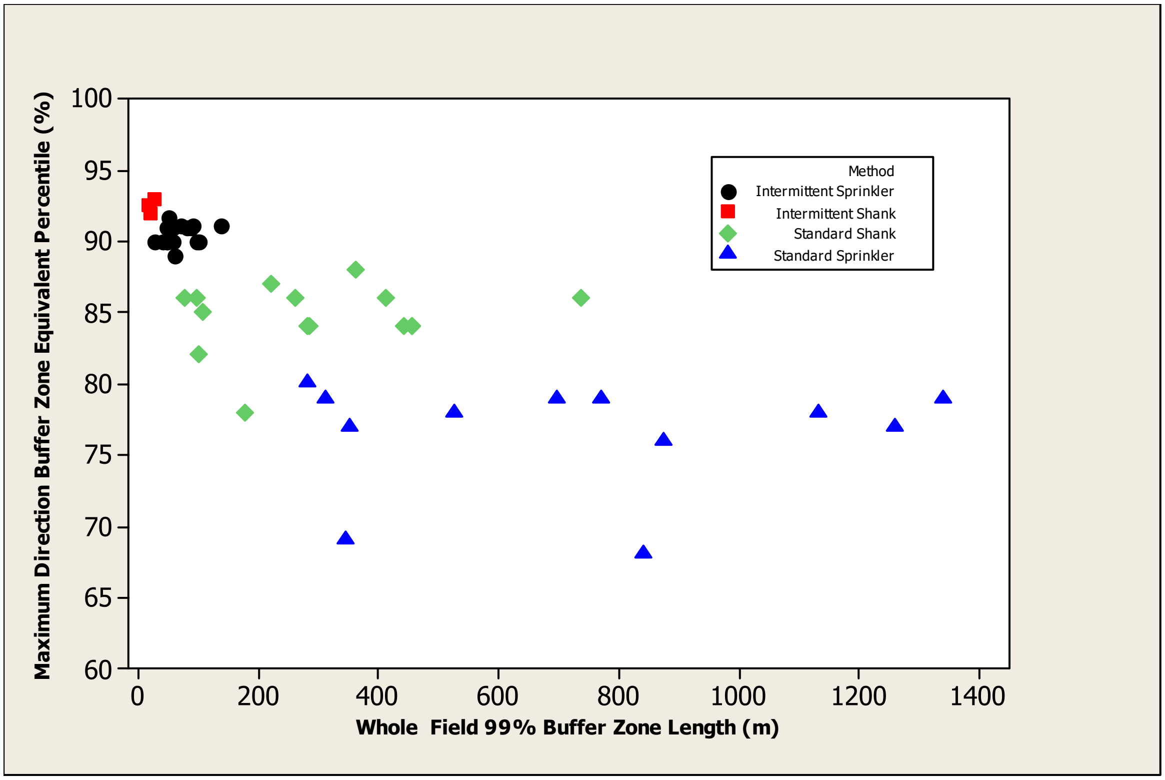


Figure 5. Relationship between the chloropicrin 99% whole field buffer zone length (m) and the equivalent maximum direction buffer zone percentile. Equivalent maximum direction percentile = individual application level protection probability = (1 – individual application buffer zone failure rate).

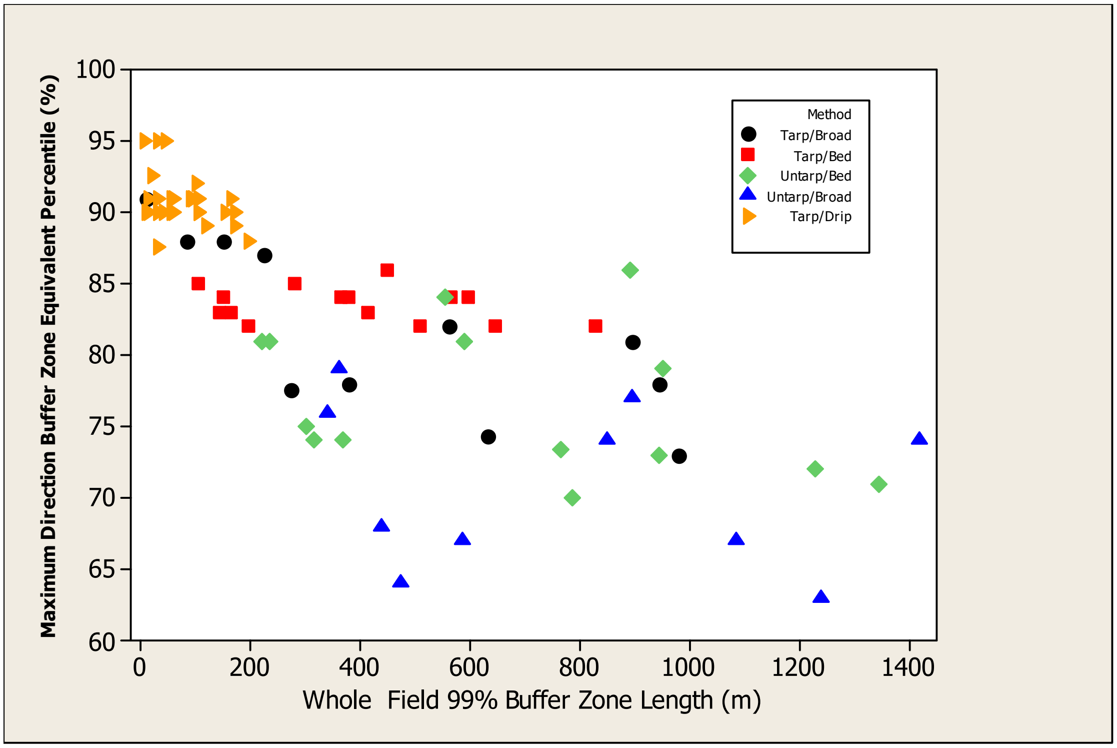
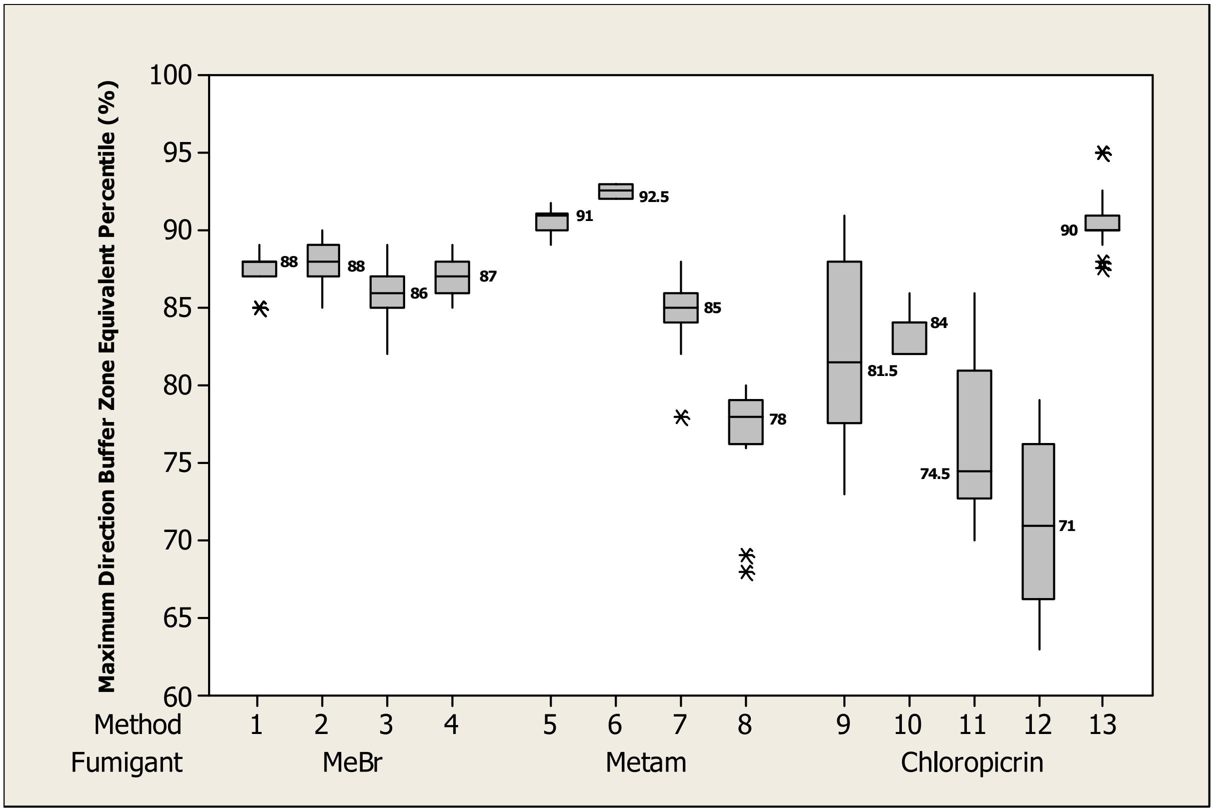


Figure 6. Summary of the maximum direction buffer zone equivalent percentiles for the 99% whole field buffer zone of application methods for methyl bromide, metam sodium and chloropicrin. The application methods within each fumigant are as follows: methyl bromide (MeBr) 1 = tarp/broadcast, 2 = tarp/bed, 3 = untarp/shallow, 4 = tarp/deep. Metam sodium (Metam) 5 = intermittent watering-in sprinkler, 6 = intermittent watering-in shank, 7 = standard shank, 8 = standard sprinkler. Chloropicrin (Chloropicrin) 9 = tarp/broadcast, 10 = tarp/bed, 11 = untarp/bed, 12 = untarp/broadcast, 13 = tarp/drip. Key to the boxplot: the median value is the line shown inside each box. The value of the median for each box is labeled next to the line. The top and both of the box indicate the lower and upper quartiles. The line (whisker) extends to the lower and upper values that are within 1.5 times the inter-quartile range. The stars indicate outlier values. Equivalent maximum direction percentile = individual application level protection probability = (1 – individual application buffer zone failure rate).



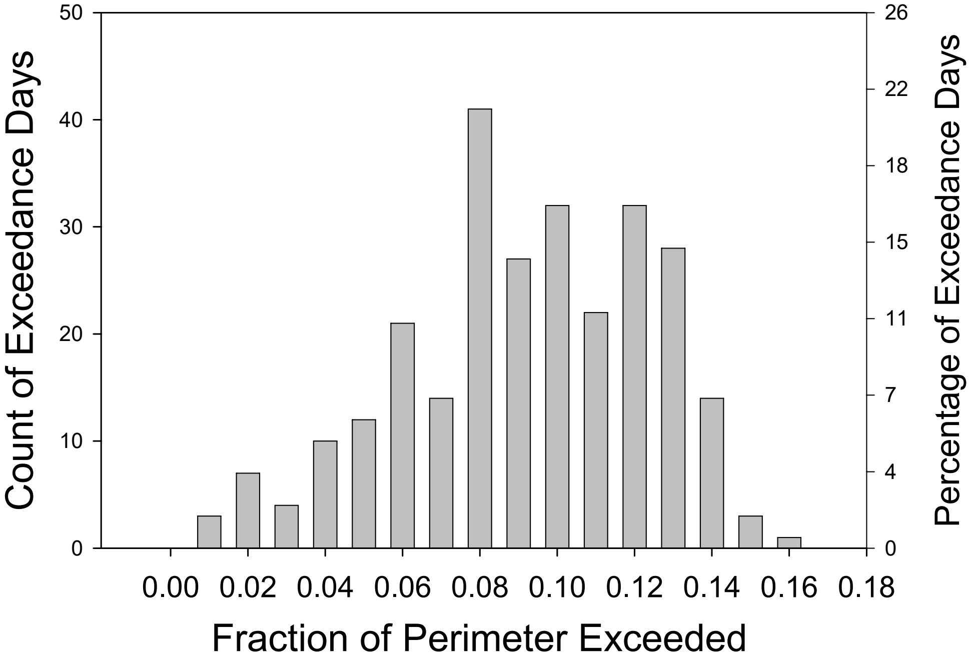


Figure 7. Fine grid, 5 acre scenario with histograms of the daily fractions of the perimeter where the concentration exceeded the reference level. The total days were 1794, of which 1523 days showed no exceedance. This figure plots the exceedances for the 271 days where 1 or more spokes showed an exceedance.

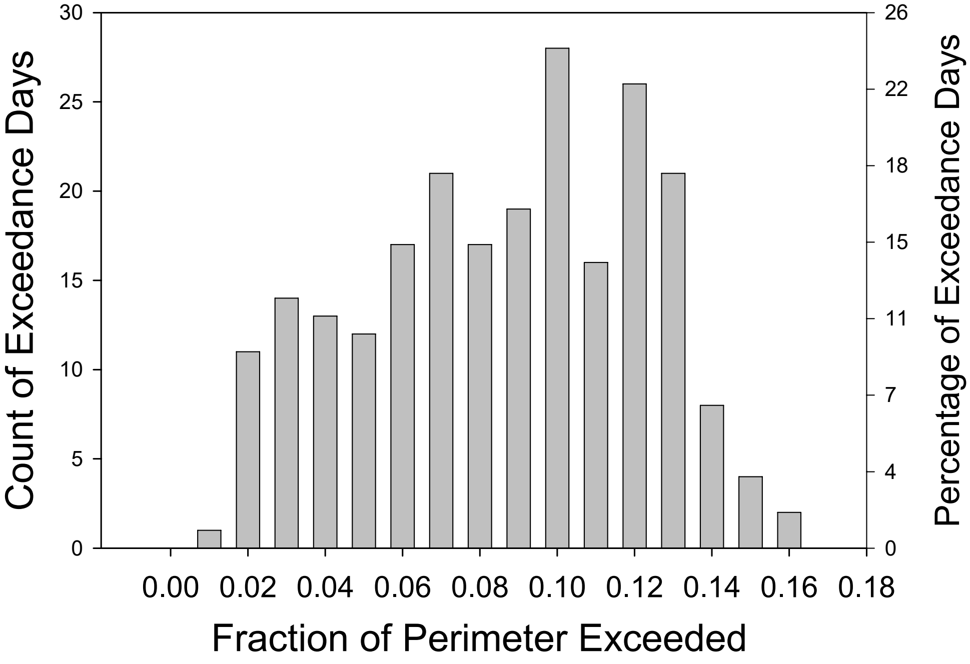


Figure 8. Fine grid, 20 acre scenario with histograms of the daily fractions of the perimeter where the concentration exceeded the reference level. The total days were 1794, of which 1564 days showed no exceedance. This figure plots the exceedances for the 230 days where 1 or more spokes showed an exceedance.

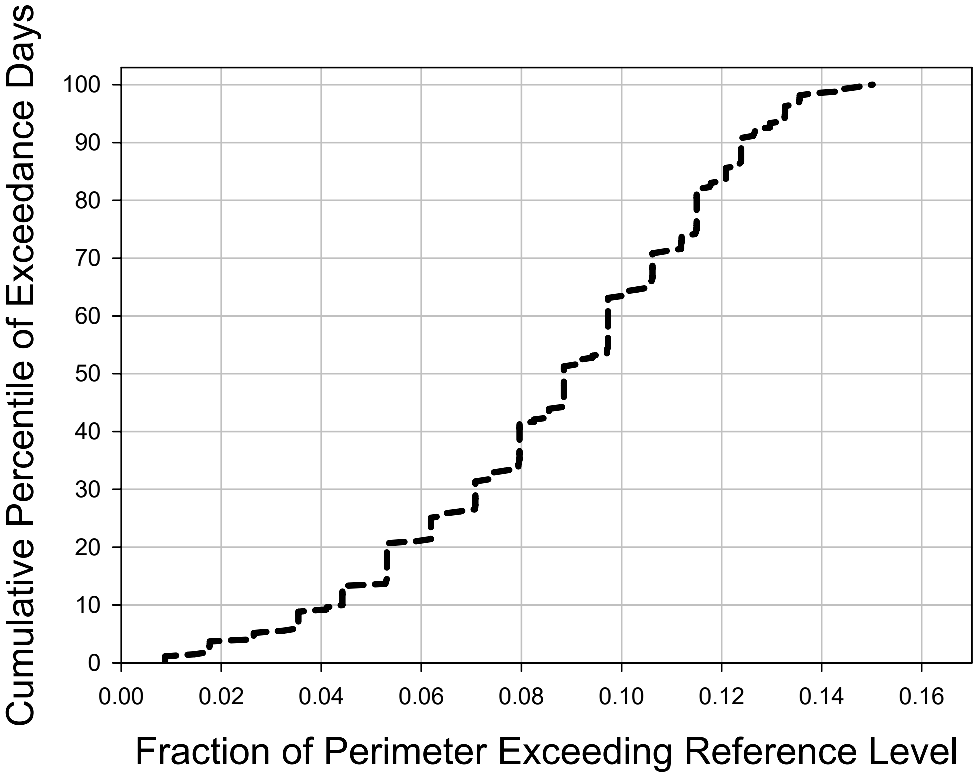


Figure 9. Cumulative distribution of perimeter length exceedances for 5 acre, fine grid scenario based on 271 days where at least one spoke exceeded the reference concentration at the buffer zone distance.

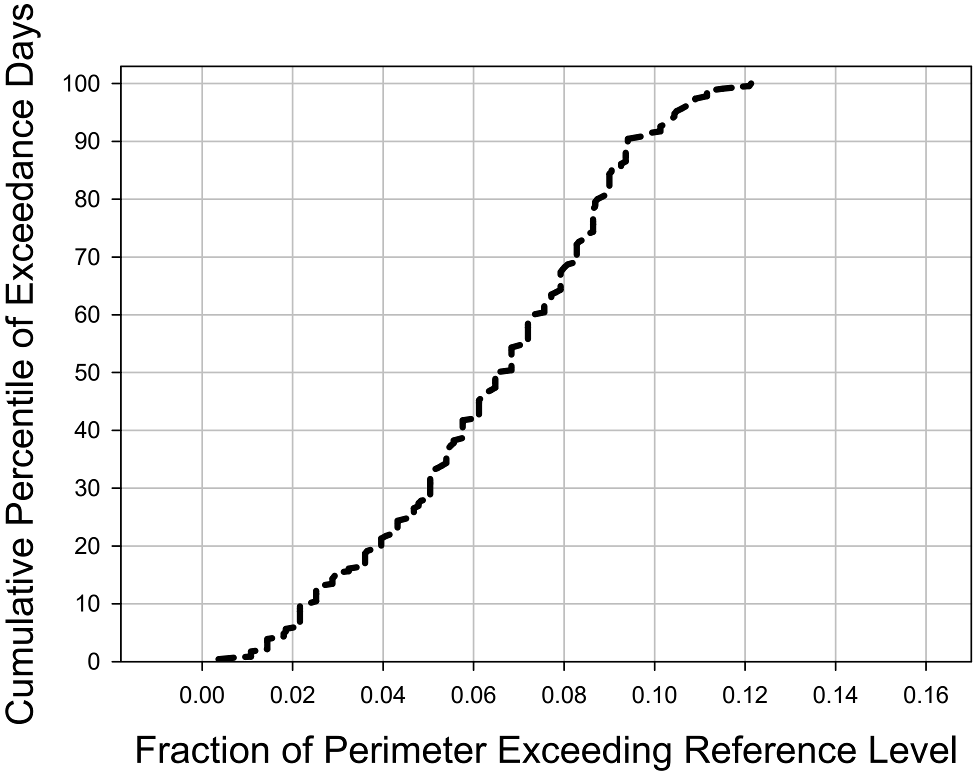


Figure 10. Cumulative distribution of perimeter length exceedances for 20 acre, fine grid scenario based on 230 days where at least one spoke exceeded the reference concentration at the buffer zone distance.