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MEMORANDUM

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SUBJECT: SCREENING LEVEL AIR CONCENTRATION ESTIMATES FOR WORKER HEALTH AND SAFETY EXPOSURE APPRAISALS

Background

The Department of Pesticide Regulation (DPR) exposure appraisals have relied exclusively on air concentrations measured in monitoring studies. However, measured air concentrations are limited in the context of estimating exposure because a measured air concentration results from a unique combination of application and meteorological conditions. The maximum air concentration associated with an application is unknown because it is unlikely that the highest air concentration present was captured by the finite set of air samplers. In addition, due to the dependence of measured air concentrations on specific application conditions, it is not possible to apply results obtained from a single study directly to other conditions. Methods have been develop using air dispersion models to generalize results from single monitoring studies so that results can be applied to other conditions.

Air dispersion models are mathematical models that describe and quantify the dispersal of pollutants in the atmosphere following release from point, line, volume, or area sources. Thus, the atmospheric processes known to disperse pollutants emitted from sources are characterized in an air dispersion model, allowing the estimation (prediction) of air concentrations at receptors located off-site around a source. In the case of soil fumigants it is only necessary to consider areas sources. More complex considerations are required to model commodity and structural fumigants.

The U.S. Environmental Protection Agency (U.S. EPA) Office of Air and Radiation and Office of Air Quality Planning and Standards administers the program which reviews and accepts candidate models as "preferred," "alternative," or "screening," and maintains air dispersion model codes. This process insures uniformity in the models and modeling procedures among users. The "preferred" model status is required for State Implementation Plan revisions for existing sources and for New Source Review and Prevention of Significant Deterioration programs (40 CFR 51, Federal Register, 2005). The "preferred" models related to DPR applications are the AMS/EPA Regulatory Model (AERMOD) (U.S. EPA, 2004) and CALPUFF (Scire et al., 2000). The "alternative" model status allows for reviewed models to be used in regulatory applications with case-by-case justification (Section 3.2, Appendix W, 40 CFR 51, Federal Register 2005). The reviewing authority in this case is DPR and the "alternative" model related to DPR applications is Industrial Source Complex Short Term Version 3 (ISCST3) air dispersion model (U.S. EPA, 1995). The ISCST3 model was a "preferred" model prior to the promulgation of the AERMOD model in December 2006 (40 CFR 51, Federal Register, 2005).

Since the 1990's, DPR has used the ISCST3 air dispersion model extensively (Johnson et al, 1999; Barry, 2000a, Johnson and Barry, 2005) to estimate off-site fumigant air concentrations. For the purposes of this project, DPR is not required to shift to either AERMOD or CALPUFF because these applications are not related to the State Implementation Plan or the Prevention of Significant Deterioration programs. In addition, the improvements gained by use of AERMOD are not implemented in the area source portion of that model. Use of CALPUFF has been considered. However, CALPUFF is a complex model that requires extensive meteorological inputs that are not readily available. While it is likely CALPUF will be integrated into the DPR modeling program in the future, at this time it is not in use.

The ISCST3 model uses a steady-state Gaussian plume dispersion equation to estimate downwind air concentrations from point, volume, and area pollutant sources. For fixed meteorological conditions, the Gaussian plume algorithm produces downwind air concentrations that are directly proportional to the emission rate (flux) of a pollutant. In addition, DPR has assumed that flux is directly proportional to the application rate (Segawa et al., 2000). The resulting proportional linkage between application rate and concentration simplifies calculations under fixed meteorological conditions.

The ISCST3 model can be used in three distinct ways: (1) the screening mode, (2) the PERFUM model, and (3) the FEMS model. For a chosen emission scenario, the screening mode produces a single air concentration estimate at a receptor (a point location at a specified distance from the source) using a single set of worst-case meteorological conditions. This means that a single downwind centerline set of air concentration estimates at various distances is the result of the analysis. Although there are differences in their approaches, the PERFUM and FEMS models are "probabilistic" in the sense that for a chosen emission scenario, historical weather data is used to produce multiple air concentration estimates at each receptor. This produces a distribution of air concentrations at a given receptor over the span of the meteorological data. Use of these distributions requires defining one or more key percentiles (e.g. 95th percentile) concentrations corresponding to key percentiles identified by risk managers.

The Worker Health and Safety (WHS) branch has chosen the screening mode for this project. This memorandum describes the method employed by DPR using air dispersion modeling to estimate screening level worst case air concentrations under the range of application methods and rates expected for a given chemical. The fumigants, iodomethane, and chloropicrin will provide examples of this method.

Throughout this memorandum the air concentrations and flux represent time weighted averages (TWA) that are either measured over a single sampling interval or are composites of shorter time intervals. Air concentration results are dependent upon sample interval duration. If fumigant air concentrations at a fixed location were measured at 1 minute intervals for 24 hours (hrs) the resulting 24 point plot would show a sharply fluctuating function with many peaks and valleys due to the intermittency with which the fumigant plume contacted the air sampler. Fumigant application site monitoring seldom uses 1 minute sampling intervals. Instead, sampling intervals of 2 to 12 hrs are employed. An air sampler at a fixed location accumulates intermittent deposits of fumigant mass during a sampling interval. The total mass collected is divided by the total volume of air pulled through the sampler during the sampling interval and this quotient become the air concentration for that sampling interval. Flux measurements are based upon air concentration measurements so the same properties apply. Thus, a single sampling interval concentration measurement represents a TWA of the peaks and valley in the hidden, high frequency concentration function during the sampling interval. The same TWA properties apply to composites of several shorter intervals of varying duration into a longer average. The longer average is constructed as an average weighted according to the individual sampling interval durations.

Methods

There are two components to the process of obtaining air concentration estimates for use in a screening level exposure appraisal: (1) generic ISCST3 simulation results which can be adapted to the specifics of an exposure scenario and (2) specific elements in the exposure scenario which are utilized to adapt the generic simulation results. The generic ISCST3 simulation results consist of downwind air concentration estimates generated using fixed meteorological conditions and using a nominal flux of 100 ug/m^2s. Sets of generic concentration estimates are produced for different acreages and meteorological condition combinations. Exposure scenario elements are used to choose appropriate acreage and meteorological conditions and to adjust the downwind air concentrations. Exposure scenario elements consist of four, interrelated kinds of parameters: (1) expected application parameters (chemical, application size, application method and rate), (2) flux estimates from field studies, (3) health threshold averaging time and possibly concentration, and (4) meteorological conditions. Each input class will be discussed below.

(1) Expected Application Parameters

These parameters are either available from use patterns for registered pesticides, or must be specified for a new pesticide that is in the registration process. Typically, the largest single day application acreage labeled or expected is simulated as a square field. The largest single day application acreage may reflect label conditions or physical limitations on the size of an application that can be made in a single day. Although other field geometries may be more common in practice, for simulation and comparison purposes the square field presents a uniform case across chemicals, application methods and rates. In addition to the largest single day application acreage, the largest allowed application rate is also used. The largest allowed application rate may be smaller than the maximum labeled rate.

The application method must be adequately described and studied in at least one reviewed field study so that a flux profile can be developed. The flux profile characterizes the progression of flux values over time following the application. The application rate used for air dispersion modeling is the "effective broadcast application rate" (Barry et al., 2004) defined as the total mass of chemical applied to a field divided by the size of the field. This method of designating the application rate removes the consideration of "treated" versus "broadcast" acres. It makes no difference whether the total mass is applied to rows or broadcast because the application is modeled as a uniform area source.

(2) Flux Estimates from Field Studies

The flux profile is typically presented as a plot or table showing the flux value observed for each averaging period of the field study. The flux profile for an application method must be developed before air dispersion modeling to estimate air concentrations under various use scenarios can be conducted. The flux profile can be developed using either the back-calculation method (Johnson et al., 1999), or a direct flux estimation method (e.g., Majewski, et al., 1995). The fully characterized flux profile will have averaging intervals that match the sampling intervals used in the field study. These averaging intervals may not match the Health Threshold averaging time. In that case additional analysis is required to obtain the flux estimates used to adjust the generic centerline concentrations. The analysis method used to obtain the centerline adjustment flux values must be fully described. The relationship between the flux profile averaging times and the time of day should be preserved in the process of adjusting the generic centerline concentrations. Thus, a day flux is used only with the day conditions centerline and a night flux is used only with the night conditions centerline. In cases of averaging intervals that span sunrise or sunset, both day and night air concentration estimates should be calculated.

(3) Health Threshold Averaging Time and Concentration

The Health Threshold averaging time must be specified in order to designate the proper averaging time for the air concentration estimates. The health threshold concentration is not always used directly in the air dispersion modeling but it is required if the exposure appraisal includes distances to specific air concentrations. If the Health Threshold averaging time is significantly shorter than the sampling intervals in the field study and the fumigant of interest has very short-term irritant properties then it may be necessary to apply a peak-to-mean adjustment (Barry, 2000b) to the estimated air concentrations. Application of the peak-to-mean adjustment can be viewed as a component of risk management and should be discussed with the exposure assessment team. Thus, the peak-to-mean adjustment is not necessarily applied simply because the flux sampling interval is longer than the desired Health Threshold Averaging Time.

(4) Meteorological Conditions

The meteorological data is considered screening level and represents reasonable worst case. The choice of screening level meteorological conditions depend upon the Health Threshold averaging time and, for averaging times shorter than 24 hrs, night versus day. For a Health Threshold averaging time of 24 hrs (e.g. methyl bromide) the screening conditions are wind speed of 1.4 m/s and atmospheric stability of slightly unstable (Class C in the Pasquill-Gifford classification scheme) (Johnson and Barry, 2005). For Health Threshold averaging times shorter than 24 hrs, day screening conditions are wind speed of 1.0 m/s and atmospheric stability class of neutral (Class D in the Pasquill-Gifford classification scheme) (Barry et al., 2004) and night screening conditions are wind speed of 1.0 m/s and atmospheric stability moderately stable (Class F in the Pasquill-Gifford classification scheme) (Barry, 2000c, Barry et al. 2004).

Example 1: Estimated Iodomethane Air Concentrations

The U.S. EPA recently granted iodomethane a conditional registration (U.S. EPA, 2007). As part of the registration process the registrant conducted eight studies to characterize the flux profile of iodomethane following application to soil by three different methods: broadcast/tarp, bed/tarp, and drip/tarp (Baker et al., 2001; Baker et al., 2002 a; Baker et al., 2002b; Baker et al., 2003; Baker et al., 2004a; Baker et al., 2004b; Baker et al, 2004c).

Iodomethane is under review for registration in California. The DPR iodomethane exposure appraisal will use off-site air concentrations that were estimated using screening air dispersion modeling. The process to produce those air concentration estimates is described and illustrated in this section. The full set of air concentration estimates developed for the WHS chloropicrin exposure appraisal are shown in Appendix A. Table 1 shows the iodomethane field studies conducted, the treated area application rate, the effective broadcast application rate, and the proportional factor needed to adjust from the effective broadcast rate in the study to the expected label application rates. Some of the field studies were conducted at application rates higher than those now labeled under the federal conditional registration. The proportion of the study effective broadcast rate can be used to adjust air concentrations to the desired effective broadcast application rate for various use scenarios. The 175 lb/acre adjustment factor is calculated by dividing 175 lb/ac by the study effective broadcast application rate.

Table 2 shows the flux estimates for three averaging times obtained from each study flux profile. The three averaging times shown (24, 8, and 1 hr) are those requested by WHS and included in the DPR iodomethane exposure appraisal. The flux estimates in Table 2 are the highest flux values obtained using the study flux profiles and a rolling average method where necessary to obtain the highest flux for each of the desired Health Threshold averaging periods (24, 8, and 1 hr). The total interval of time associated with each TWA flux is shown in parentheses in Table 2. The TWA intervals vary because studies do not always have sampling interval durations that match the Health Threshold averaging time. Ideally, the TWA flux should be over a period equal to or shorter than the desired Health Threshold averaging time. For a constant flux, an air concentration measured at a particular receptor is a function of averaging time. Under those conditions, air concentrations taken over shorter intervals will be higher relative to those taken over longer intervals. This phenomenon is well described in air dispersion theory literature (Csanady, 1973; Pasquill, 1974)

To calculate the 24 hr screening air concentration estimates the appropriate flux estimates were obtained by taking rolling weighted averages until the largest 24 hr flux was obtained. The interval durations for the 24 hr flux were between 19 and 24 hrs. In all cases the first 24 hrs yielded the highest 24 hr TWA flux. For the 8 hr air concentration estimates the flux estimates were obtained by taking rolling weighted averages of sampling periods between 2 and 4 hrs duration. Thus, the 8 hr flux estimates are based on 6 hr to and 8 hr weighted averages.

To calculate 1 hr screening air concentrations it is necessary to estimate maximum 1 hr flux. Obtaining 1 hr flux estimates can be problematic. In most studies the sampling intervals will be longer than 1 hr, and commonly no smaller than 4 hrs. However, several of the Iodomethane studies had early sampling intervals of 2 or 3 hrs. Thus, the 1 hr air concentration estimates flux estimates measured in sampling intervals ranging from 2 to 4 hrs were used directly. An alternative is to use a “peak-to-mean” adjustment to account for estimating a shorter duration concentration from longer duration concentrations (Barry, 2000b). WHS has opted not to use the peak to mean adjustments for the 1 hr modeled air concentrations because iodomethane is not an acute irritant (unlike chloropicrin or other irritants) and the averaging times of the sampling intervals were judged close enough to 1 hr to use directly from the study results.

The process of producing the 24 hr screening air concentration estimates for the Manteca broadcast/tarp application method and a 40 acre square field is illustrated in Table 3. The remaining estimates for other application methods and locations can be found in Appendix A. The third column of Table 3 shows the generic downwind centerline air concentrations at 6 distances between 3.04 m (10 ft) and 760 m (2500 ft) from the application edge. These air concentrations were produced at a receptor height of 1.2 m representing the human breathing zone using the ISCST3 model with inputs of a 40 acre square source, generic flux (100 ug/m^2sec), the standard weather data for 24 hrs (1.4 m/s wind speed and C stability; see Johnson and Barry, 2005). These generic downwind centerline air concentrations can be used for any fumigant that uses a 24 hr Health Threshold averaging time. Only the fumigant/application method combination specific adjustment for the flux and application rate is needed to produce scenario specific air concentration estimates.

For this Manteca Broadcast/Tarp application method iodomethane study, the adjustment factors are as follows (see Table 2, row 2):

The field study has a 24 hr TWA flux estimate = 160.2 ug/m^2s

The flux adjustment factor (multiplier) for the generic air concentrations is calculated as:

$$(160.2 \text{ ug/m}^2\text{s}) / (100 \text{ ug/m}^2\text{s}) = 1.602$$

This multiplier is applied to the downwind centerline concentrations as follows:

3.04 m generic downwind centerline air concentration = 2589.13 ug/m^3

3.04 m 242 lb/ac broadcast/tarp downwind centerline air concentration =

$$(1.602)(2589.13 \text{ ug/m}^3) = 4147.8 \text{ ug/m}^3$$

The 4147.8 ug/m^3 result is shown in column 4 of Table 3.

The next application rate factor is calculated.

The 175 lb/ac application rate adjustment =

$$(175/242) = 0.72$$

The 3.04 m 175 lb/ac broadcast/tarp downwind centerline concentration =

$$(0.72)(4147.8) = 2986.4$$

It is recommended that the air concentration estimates be rounded to 2 significant figures for use in the exposure appraisals.

The generic downwind centerline air concentrations for averaging times shorter than 24 hrs use the standard weather conditions for day (1.0 m/s and D stability) and night (1.0 m/s and F stability). The relationship between the flux profile as it was developed in the field study and the diurnal cycle is preserved. Thus, to produce the estimates, the highest day averaging time flux is matched with the day standard weather conditions, while the highest night averaging time flux is matched with the night standard weather conditions. The scenario producing the highest off-site air concentration is emphasized in the air concentration estimation. As an example of the shorter averaging time, Tables 4 and 5 show the day 1 hr TWA and the day 8 hr TWA (respectively) iodomethane air concentration estimates for the Manteca study.

The Generic day 1 hr air concentrations (Table 4) are produced with the standard day meteorological conditions (D-stability and 1 m/s wind speed) and generic flux of 100 ug/m^2sec.

The calculations are as follows:

The Manteca broadcast/tarp field study has a 1 hr TWA flux estimate = 481.0 ug/m^2sec (Table 2).

The flux adjustment factor (multiplier) is calculated as:

$$(481.0\ ug/m^2s) / (100\ ug/m^2s) = 4.810$$

This multiplier is applied to the downwind centerline concentrations as follows:

3.04 m generic downwind centerline air concentration = 5181.70 ug/m^3

3.04 m 242 lb/ac broadcast/tarp downwind centerline air concentration =

$$(4.810)(5181.70\ ug/m^3) = 24924.0\ ug/m^3$$

The 24924.000 ug/m^3 result is shown in column 4 of Table 4.

The results for the 175 lb/ac application rate are shown in column 5 of Table 4.

The 175 lb/ac application rate adjustment =

$$(175/242) = 0.72$$

The 3.04 m 175 lb/ac broadcast/tarp downwind centerline concentration =

(0.72)(24924.0) = 17945.3

The Generic day 8 hr air concentrations are produced with the standard day meteorological conditions (D-stability and 1 m/s wind speed) and generic flux of 100 ug/m^{2}sec. The Generic Day 8 hr air concentrations are the same as the Generic Day 1 hr TWA concentrations because the meteorological conditions and the generic flux are the same. The difference in final screening air concentrations is accounted for in the flux estimates, which are measured over different averaging times. The calculations are as follows:

The field study has an 8 hr flux estimate = 313.7 ug/m^{2}sec (Table 2).

The flux adjustment factor (multiplier) for the generic air concentrations is calculated as:

(313.7 ug/m^{2}s) / (100 ug/m^{2}s) = 3.14

This multiplier is applied to the downwind centerline concentrations as follows:

3.04 m generic downwind centerline air concentration = 5181.700 ug/m^3

3.04 m 242 lb/ac broadcast/tarp downwind centerline air concentration =

(3.14)(5181.70ug/m^3) = 16270.5 ug/m^3

The 16270.500 ug/m^3 result is shown in column 4 of Table 5.

The next application rate factor is calculated.

The 175lb/ac application rate adjustment =

(175/242) = 0.72

The 3.04m 175lb/ac broadcast/tarp downwind centerline concentration =

(0.72)(16270.5) = 11714.8

Estimated air concentrations for all 8 iodomethane field studies under all meteorological and averaging time scenarios can be found in Appendix A.

Example 2: Chloropicrin

The full set of air concentration estimates developed for the WHS chloropicrin exposure appraisal are shown in Appendix B. Flux profiles for 5 application methods are available: broadcast/untarp, bed/untarp, bed/tarp, broadcast/tarp, and bed/drip/tarp. (Beard, 1996; Rotandardo, 2004). The broadcast/tarp application method has three flux profiles from three separate field studies in Arizona, Washington, and Florida. The Health Threshold averaging times for the chloropicrin exposure appraisal are 24, 6, and 1 hr. A summary of the field study application methods and rates and the flux estimates used for the chloropicrin exposure appraisal are shown in Table 6.

The process of producing the night 1 hr chloropicrin air concentration estimates for the Arizona broadcast/tarp application method and a 40 acre square field is illustrated in Table 7. The estimates for other application methods and locations can be found in Appendix B. The shortest sampling interval in the Arizona broadcast/tarp field study was 6 hrs. Consequently the 1 hr air concentration estimation will begin with results for the 6 hr averaging time. Then the peak-to-mean adjustment is made to the 6 hr air concentrations to obtain the 1 hr air concentration estimates. The WHS branch has requested the use of the peak-to-mean adjustment because chloropicrin is an irritant at low concentrations.

The third column of Table 7 shows the generic night 6 hr downwind centerline air concentrations at 6 distances between 3.04 m (10 ft) and 760 m (2500 ft) from the application edge. These air concentrations were produced at a receptor height of 1.2 m (representing the human breathing zone) using the ISCST3 model with inputs of a 40 acre square source, generic flux (100 ug/m^2sec), the standard weather data for 6 hr night conditions (1 m/s wind speed and F stability). These generic downwind centerline air concentrations can be used for any fumigant that uses a 6 hr threshold averaging time, and, in fact were used to produce the chloropicrin night 6 hr air concentration estimates (see Appendix B). These concentrations are considered 6 hr concentrations because the averaging time on the flux estimate is 6 hours. The 6 hr sampling interval is the shortest interval in the Beard et al. (1996) study. Hence, in this case it is used as the basis to generate 1 hr air concentrations using peak-to-mean adjustment methods (Barry, 2000b).

For this Arizona Broadcast/Tarp application method chloropicrin study, the adjustment factors are as follows (see Table 7):

The field study has a night 6 hr flux estimate = 30.15 ug/m^2sec

The 332 lb/acre application rate flux adjustment factor (multiplier) for the generic air concentrations is calculated as:

$$(30.15 \text{ ug/m}^2\text{s}) / (100 \text{ ug/m}^2\text{s}) = 0.3015 \text{ (Table 6)}.$$

This flux adjustment multiplier is applied to the 6 hr generic downwind centerline concentrations as follows:

3.04 m generic downwind centerline 6 hr air concentration = 8329.80 ug/m^3

3.04 m 332 lb/ac broadcast/tarp downwind centerline air concentration =

$$(0.3015)(8329.80 \text{ ug/m}^3) = 2511.4 \text{ ug/m}^3$$

The night 6 hr air concentration estimate of 2511.4 ug/m^3 is shown for the downwind distance of 3.04 m in column 4 of Table 7. The next step is to develop the 1 hr air concentration estimate for this application rate by applying the peak-to-mean adjustment to the 6 hr estimates as follows:

The peak-to-mean adjustment for 6 hrs to 1 hr = 2.45

This multiplier is applied to the 6 hr air concentration estimates in column 4 of Table 7 as follows:

$$(2.45)*(2511.4) = 6153.0$$

Results of this adjustment are shown in column 5 of Table 7.

The next application rate is calculated.

The estimates for 350 lb/ac application rates are made as follows:

$$\text{application rate adjustment} = (350/332) = 1.0542$$

This adjustment is applied to the 332 lb/ac 6 hr TWA concentrations in column 4 of Table 7:

$$(1.0542)*(2511.4) = 2647.6$$

Results are shown in Column 6 of Table 7. The peak-to-mean adjustment of 2.45 is then applied to the 350 lb/acre 6 hr air concentration estimates shown in Column 6 to produced the 1 hr air concentration estimates:

$$(2.45)*(2647.6) = 6486.5$$

The 1 hr air concentration estimates for 350 lb/ac are shown in Column 7 or Table 7.

It is recommended that the air concentration estimates be rounded to 2 significant figures for use in the exposure appraisals.

Summary

These air dispersion modeling methods can be used to produce worst case exposure appraisal air concentration estimates for any fumigant that has a developed flux profile. The Health Threshold averaging time, application rates, and maximum field size are fumigant specific. However, the basic procedures would be similar.

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