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SUBJECT: EVALUATION OF THE AIR DISPERSION MODELING TOOL SOFEA2

Background:

The air dispersion modeling tool SOFEA2, developed by Dow AgroSciences LLC (Dow), has been the subject of CDPR review since February 2014. The focus of the SOFEA2 modeling tool is estimating air concentrations of 1,3-Dichloropropene (1,3-D) associated with applications of the fumigant. The SOFEA2 model has been revised several times since the earliest version (dated December 31, 2013) was submitted for review. New data volumes were submitted for review following each revision. Various errors in the SOFEA2 model have been corrected with each new version. Dow also conducted a 14.5 month air monitoring study to collect measured air concentrations with the objective to validate the SOFEA2 model (Rotondaro and van Wesenbeeck, 2012). EM staff performed a complete review of the SOFEA2 model and the DOW validation analysis in data volume 50046-0210 (ID263794) (Johnson, 2014). The following technical deficiencies were noted:

1) SOFEA2 under estimates higher air concentrations

The Johnson (2014) evaluation of the March 21, 2014 version of SOFEA2 was confined to air concentrations measured and modeled at the 9 air monitoring locations in the center of the 9 townships from the Rotondaro and van Wesenbeeck, (2012) study. Based upon that analysis, Johnson (2014) concluded that "…SOFEA2 does a relatively poor job of estimating concentrations in both time and space."

2) SOFEA2 incorporates a version of the CHAIN2D model called VEFE which was assumed to have been used to generate the air concentrations presented in vol 50046-0210.

This current evaluation reviews the most recent version of SOFEA2 that includes: 1) corrections and improvements related to the Johnson (2014) review, 2) a new approach to more fully account for the effect of meteorological variables on air concentrations, and 3) additions to SOFEA2 to account for the influence of applications made outside of the 9 township area monitored by Dow on the measured and modeled 1,3-D air concentrations.

Evaluation:

The SOFEA2 model will be used as a prospective modeling tool. Specifically, the SOFEA2 model will be used to generate annual average air concentrations associated with the use of 1,3-D over many years in a region. The minimum geographic area of interest is the Public Land Survey System “township” (survey township) which is a 6 mile by 6 mile square parcel of land in California. The simulated annual average 1,3-D air concentrations are then used in risk analysis. Thus, the evaluation of the SOFEA2 model is in the context of how well the SOFEA2 model can be argued to capture the potential high concentrations associated with the use of 1,3-D. Air concentrations at any one specific point within a township is not of interest because the exact location of air concentrations within the township is not important in the risk analysis.

The Dow monitoring study (Rotondaro and van Wesenbeeck, 2012) was conducted over a 3 x 3 township area. This is a geographic scale of 18 miles by 18 miles. Nine air samplers were employed within this monitoring domain - one air sampler in the center of each township. Considering the scale of the modeling domain, this is an extremely sparse sampling set with which to validate the SOFEA2 model using air concentrations matched in space and time. However, the nine air sampler results can be used to explore whether SOFEA2 is generating maximum air concentrations sufficiently high to be argued that the worst case air concentrations have been captured. Due to the sparse sampling, it can be assumed that the maximum air concentration during the monitoring study was not captured by the air samplers. Therefore, the maximum air concentration is unknown and likely larger than the maximum measured air concentration. Furthermore, the design of the Dow monitoring study necessitates keeping all 9 townships together as a single domain of interest. The questions then are: 1) Does the model produce air concentrations at least as high as those measured and 2) Does the model produce annual average 1,3-D air concentrations that reflect the actual distribution of annual 1,3-D air concentrations during the monitoring study. The answers to both of these questions are highly dependent on the density of the receptor grid used to run the SOFEA2 model. A 9 receptor modeling grid that only represents the locations of the 9 air monitored locations within the 9 township (18 mile by 18 mile) area is not sufficient to evaluate the SOFEA2 model performance in the context of a prospective risk assessment scenario. Modeling with such a sparse receptor grid is extremely unlikely to adequately characterize the actual distribution of air concentrations in 9 township model domain.

The Dow monitoring was conducted as continuous 72-hr sampling periods over 14.5 months. This model evaluation will examine the period average, which is a 14.5 month average for two reasons: 1) the SOFEA2 model would not run to completion (this will be discussed further below) and 2) the end use of the data is the risk assessment process using the annual averages. The 14.5 month averages can be used as a surrogate for the annual average in this initial model evaluation.

An independent SOFEA2 model run at CDPR was used to evaluate the model. Results presented in the data volume guided the CDPR evaluation but are not the focus of this evaluation. As stated earlier, the distribution of 1,3-D air concentrations generated by the SOFEA2 model is highly dependent upon the density of the receptor grid. For multi-year prospective model runs in a 3x3 township model domain DOW has used a grid of 10,000 receptors (100x100 receptor frame) with a resulting spacing between receptors of about 290m (the data volume on page 23 states 11,664 receptors but that receptor grid includes extra receptors along the edges due to a bug in the receptor generating algorithm. That bug will be fixed in the next version of SOFEA). Using a 10,000 receptor grid should continue to be the practice for prospective model runs. For the DOW validation run, reported in the data volume, a receptor grid of 2500 receptors (50x50 receptor frame) spaced approximately 580 m apart was used. Initial evaluations using contour plots in SURFER software indicate that the 580 m receptor spacing is not sufficient to characterize the highest concentrations produced by the SOFEA2 model. The focus of SOFEA model validation has been whether the SOFEA2 model is sufficiently capturing the highest air concentrations. The validation model runs are retrospective rather than prospective so a very dense prospective receptor grid is not initially required. A 10,000 receptor grid generates a very large output file and is not absolutely necessary if a less fine grid of receptors spaced a little farther apart shows the SOFEA2 model captures the magnitude of the air concentrations in the 9 township area. Thus, for the initial validation a CDPR SOFEA2 run was performed using 5660 receptors (75x75 receptor frame) spaced approximately 400 m apart.

The actual CDPR model run was conducted outside of the SOFEA2 GUI because the SOFEA2 model would not run the 5600 receptor validation run to completion. The post-processing portion of the SOFEA2 run did not complete, despite many attempts to locate and fix errors that might be causing the problem. There are some serious bugs in the SOFEA2 GUI that must be corrected before this model can be used routinely at CDPR. However, this validation of SOFEA2 is a “proof of concept” with the objective being: does the ISCST model, using the SOFEA2 generated input file and the Merced weather file with the mixing height algorithm, produce air concentrations that reflect the conditions observed in the 3x3 township area monitored by DOW for 14.5 months. The post processing done by SOFEA2 after the ISCST run is not needed to achieve this objective. SOFEA2 post processing includes reporting for the entire 14.5 month period the 1 hr air concentrations at each receptor, finding the 72 hour air concentrations for each receptor, and presenting various graphical analyses. All the post processing is conducted in Excel. The post processing results are not necessary to demonstrate the proof of concept condition has been met. Thus, the procedure to obtain the output was as follows: 1) generate the 5660 receptor grid within SOFEA2, 2) run the SOFEA2 model in validation mode to obtain the ISCST input files needed for the run, 3) run the ISCST model in a separate folder using the input files generated by SOFEA2 with the mixing height corrected weather file, 4) analyze both the weather file and the ISCST period average output file.

Analysis of the mixing height corrected weather file revealed two significant errors in the DOW processing of the weather data: 1) the stability classes are not correctly assigned in some cases, and 2) the mixing heights are miss-assigned by the mixing height algorithm.

Briefly, stability classes and mixing height characterize the turbulence and degree of vertical mixing in the atmosphere. There are 6 Pasquill stability classes categorized in classes from 1 to 6. Stability class 1 is the most unstable (the most vertical mixing), while stability class 6 is the most stable (the least vertical mixing). The progression from stability class 1 through 6 depends on the angle of the sun (time of day), degrees of cloud cover, and the wind speed. Stability classes 1 – 4 occur during the day. Stability classes 4-6 occur at night. The Pasquill stability classes are used by the ISCST3 model. The mixing height is defined as the height above ground within which the atmosphere can mix vertically (Turner, 1994). The higher the mixing height, the greater the potential to disperse a pollutant, all other factors held constant.

Table 1 shows a summary of stability class by hour of the day. Stability classes 1(very unstable) and 2 (unstable) are characteristic of warm, sunny days late in the morning into early afternoon. The Solar elevation angle required for stability class 1 is an angle equal to or greater than 60 degrees above the horizon (Zanetti, 1990). Stability class 2 requires a solar elevation angle between 35 degrees and 60 degrees above the horizon. Even at the summer solstice of June 21 the solar angle at 1000 hrs is 62 degrees, just satisfying solar elevation conditions for stability class 1. Therefore, stability class 1 should not occur earlier than 1000 hrs. The same solar elevation requirements must be met in the late afternoon. In addition, the wind speed cannot be greater than 3 mph together with the solar elevation of 60 degrees or greater for a stability class 1 to be assigned to an hour. Yet, Table 1 shows many hours of stability class 1 both early in the morning and late in the afternoon. Stability class 2 also is assigned in hours where it clearly cannot occur on the environment. Stability classes 5 and 6 should only occur when the sun is below the horizon. Yet stability class 5 occurs in every hour and stability class 6 occurs in 23 of the 24 hours of the day. The mistakes in stability class assignment will tend to reduce the air concentrations estimated by SOFEA2 because there are too many hours with very unstable and unstable atmospheric conditions. The mistakes in assignment of stability classes 5 and 6 affect less hours than stability classes 1 and 2. Therefore, with respect to model validation this would tend to cause the match of measured to modeled showing that the SOFEA2 model underestimates the air concentrations. A quick check of the Merced weather file shows that stability classes change by more than one class per hour. This cannot be allowed (Johnson et al., 1999). The stability class algorithm must also be corrected so that stability classes do not change by more than one stability class per hour. For example, just before dawn if an hour is assigned stability class 6, the next hour must be 5 and the hour after that stability class 4.

Table 1. Summary of stability class assignment by hour in the MERC2010_2012_MH.met file supplied by Dow AgroSciences.

Hour	Stability Class						Total
	1	2	3	4	5	6	
0100	0	0	0	51	65	630	746
0200	0	0	0	48	62	636	746
0300	0	0	0	41	84	621	746
0400	0	0	0	53	66	627	746
0500	0	0	0	47	70	629	746
0600	150	5	0	47	88	456	746
0700	150	121	22	81	145	227	746
0800	151	283	89	150	47	26	746
0900	154	332	170	63	23	4	746
1000	188	399	110	44	2	3	746
1100	311	295	111	25	2	2	746
1200	367	252	97	28	1	1	746
1300	390	221	102	31	1	1	746
1400	395	218	98	34	0	1	746
1500	356	239	111	38	2	0	746
1600	301	268	135	40	1	1	746
1700	226	310	164	42	4	0	746
1800	176	327	164	53	6	20	746
1900	155	142	111	109	31	198	746
2000	146	26	57	154	75	288	746
2100	0	0	19	151	123	453	746
2200	0	0	0	123	103	520	746
2300	0	0	0	72	121	553	746
2400	0	0	0	55	88	603	746
Total	3616	3438	1560	1580	1210	6500	17904

The Dow mixing height adjustment algorithm is invoked when wind speed is 1.0 m/s (or less but wind speeds less than 1.0 m/s are set to 1.0 m/s). However, the adjustment should also be dependent upon the solar angle and/or the solar radiation. The Dow mixing height adjustment algorithm clearly does not distinguish between night and day hours (Table 2). This leads to the lowest median mixing height occurring during calm wind conditions in daylight hours. This is not true in the environment (Schnelle and Dey, 2000). In fact, calm winds and daylight hours combine to produce some of the highest mixing heights. Wind speeds of 1.0 m/s during the day assigns stability class 1 (very unstable). Very unstable atmospheric conditions have the highest mixing heights of the day.

Thus, the main issues with the Dow mixing height adjustment algorithm are:
1) Stability classes 1,2, and 3 should not have a mixing height adjustment at all.
2) The lowest mixing heights should happen predominantly at night or at the transition hours around sunset and/or sunrise.
3) Stability class 6 should have the lowest median mixing height.

Table 2. Summary of adjusted mixing height by hour in the MERC2010_2012_MH.met file supplied by Dow AgroSciences.

Hour	Stability Class						Total
	1	2	3	4	5	6	
0100	*	*	*	*	12.80	16.40	16.35
0200	*	*	*	*	24.20	17.30	17.40
0300	*	*	*	*	8.10	15.80	15.80
0400	*	*	*	*	23.00	16.65	16.95
0500	*	*	*	34.00	24.90	17.80	18.25
0600	31.10	19.60	*	20.30	30.10	10.20	18.10
0700	31.20	17.50	32.30	28.20	25.15	4.70	16.90
0800	31.25	8.90	28.20	24.40	7.65	1.95	16.35
0900	29.50	9.00	17.40	11.80	2.00	1.60	13.20
1000	29.05	7.40	15.15	1.95	*	*	11.80
1100	27.40	7.80	1.85	*	*	*	13.20
1200	18.80	4.10	*	*	*	*	13.40
1300	18.40	5.10	*	*	*	*	13.50
1400	17.40	4.00	*	*	*	*	9.60
1500	16.80	4.50	*	*	*	*	7.50
1600	19.20	5.60	*	*	*	*	7.40
1700	22.95	6.30	5.20	*	2.80	*	9.60
1800	19.90	5.70	7.15	*	*	2.10	6.90
1900	30.00	7.85	2.60	2.30	5.20	7.10	7.90
2000	31.90	31.30	11.75	5.70	2.05	7.30	10.20
2100	*	*	*	12.70	5.70	13.20	12.70
2200	*	*	*	31.30	12.50	13.45	13.60
2300	*	*	*	*	24.15	13.35	13.60
2400	*	*	*	23.70	2.00	14.15	13.90
Total	27.4	7.3	10.45	15.85	19.35	13.3	14.4

*No hours

The issues with stability class assignment and the mixing height adjustments prevent a firm conclusion with respect to the ISCST validation scenario modeling results. The stability class errors would tend to decrease the modeled air concentrations. The mixing height adjustment errors would likely increase the modeled air concentrations during the day but decrease them at night, relative to if they mixing height were correctly assigned to the same adjusted hours. As a result of these errors only a preliminary assessment of the modeled validation scenario air concentrations can be given.

As stated above, the SOFEA2 model itself would not run to completion. The SOFEA2 model did run the ISCST model to completion for the validation run but would not successfully perform the post processing. As a result of the SOFEA2 model "bombing" during the post processing, the output files produced by the ISCST model run did not get closed and, thus, were unavailable for analysis. The SOFEA2 post processing, while interesting, is not needed for the initial validation. SOFEA2 did successfully generate the input files needed to run the ISCST model outside of SOFEA2. For the purposes of evaluating the annual (or 14.5 month period) averages it is sufficient to use the modeling results directly from the ISCST model. No additional post processing is required. Table 3 summarizes the measured and modeled 14.5 month averages for each of the 9 monitored locations. All 9 modeled period averages for the monitored locations were within a factor of 2 of the measured 14.5 month measured air concentrations. The simplest metric to evaluate an air dispersion model is to compare the ratio of measured to modeled air concentrations. For regulatory purposes, an air dispersion model is considered "acceptable" if modeled air concentrations are within a factor of 2 of the measured air concentrations (Pratt et al., 2004).

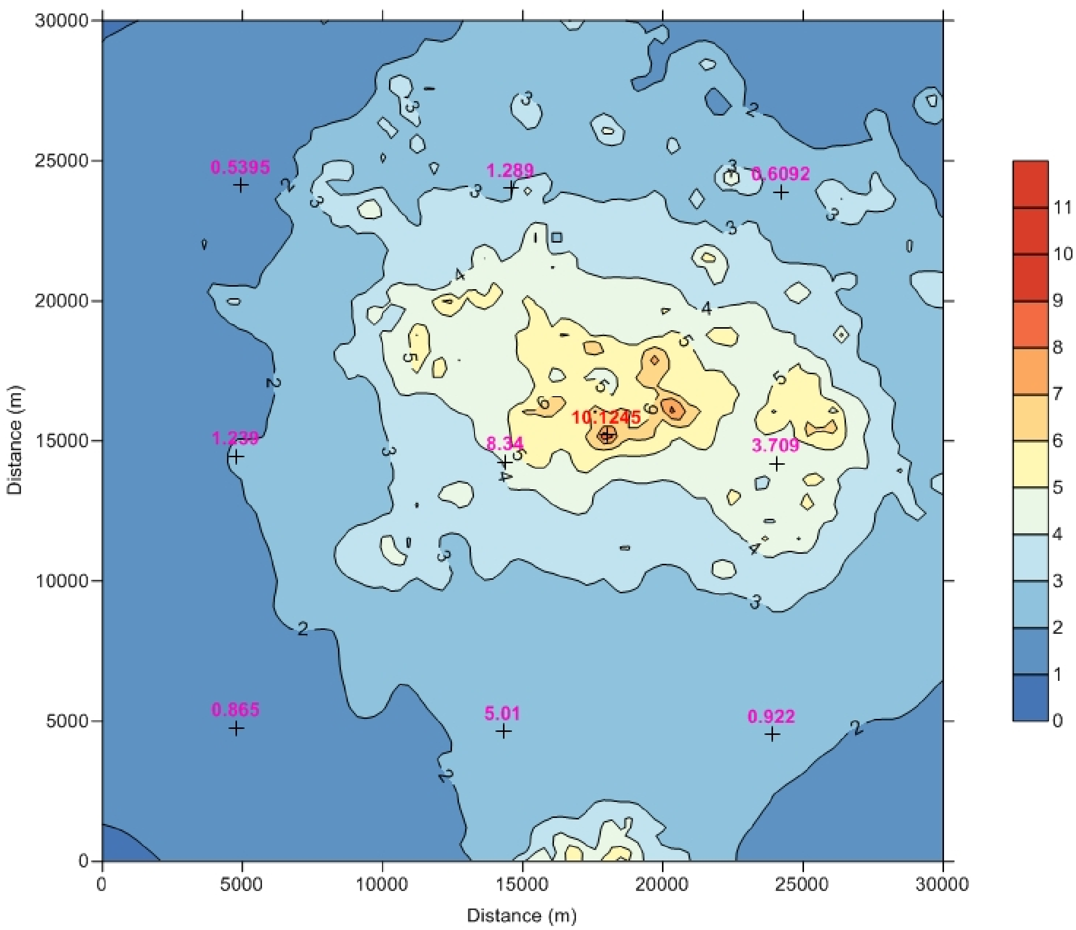
Table 3. Comparison of measured and modeled 1,3-D air concentrations (ug/m^3)

Township ID	14.5 month measured average air concentration (ug/m^3)	14.5 month modeled average air concentration (ug/m^3)	Measured/Modeled
1	0.8650	1.5278	0.57
2	5.0100	2.5171	1.99
3	0.9220	2.2478	0.41
4	1.2390	1.9790	0.63
5	8.3400	4.2815	1.95
6	3.7090	4.1197	0.90
7	0.5395	1.7330	0.31
8	1.2890	3.0171	0.43
9	0.6092	2.4413	0.25

The USEPA modeling guidelines acknowledges that air dispersion models are better at estimating longer term average air concentrations than short term (USEPA, 2005). In addition, air dispersion models can be expected to reasonably match the magnitude of the maximum concentrations in a given area over a chosen period of time but cannot be expected to match exact locations (USEPA, 2005). This is due to uncertainties in model inputs. For example, errors in location of a plume due to meteorological data uncertainties and other data input errors can cause a 50% or more error in the estimation of an air concentration at a fixed location (Pasquill, 1974). Figure 1 shows the contour plot of ISCST modeled air concentrations for the validation scenario. It should be noted that these results are highly dependent upon the receptor grid density (as discussed above).

The results in Figure 1 are for the 5660 receptor grid. If the 10,000 receptor grid had been used it is likely even higher and more numerous maximum modeled air concentrations would have been found. The maximum measured air concentration of 8.34 ug/m^3 was exceeded by the modeled receptor concentration of 10.12 ug/m^3 at 2.3 miles from the measured location. A second model receptor showed a maximum modeled air concentration of 8.58 ug/m^3. The contour plot shows that there are several areas in the model domain where the modeled concentrations are in the 8 ug/m^3 range. Also shown is that some measured locations are underestimated and other are over estimated. But in the context of the regional concentrations the ISCST Merced validation scenario run captures the measured maximum air concentrations, just not in the exact locations where they were measured. The effect of the 1,3-D applications that were made just outside the 3 x 3 township area can be seen on the lower end of the plot. This demonstrates why it is important to include those applications both in the Merced validation scenario and prospective SOFEA2 runs.

Figure 1. Contour plot of ISCST modeled Merced validation scenario 14.5 month period average 1,3-D air concentrations (ug/m^3). Black crosses are the locations of the monitored air concentrations. Purple text are the measured 14.5 month 1,3-D air concentrations (ug/m^3). This axes show the 18 mile by 18 mile area as defined by the Dow study (in meters for ISCST modeling purposes), with the southwest corner as (0 m, 0 m). This coordinate system is not GIS based, instead it is referenced for the ISCST model with respect to the southwest corner of the model domain.



Comparing the distribution of measured 1,3-D concentrations to the modeled 1,3-D concentrations directly is problematic because only 9 locations were monitored. The monitoring grid was extremely sparse. Thus, the distribution of air concentrations fit to the measured values appears to over-estimate what the highest measured 1,3-D air concentrations would have been had a more comprehensive monitoring network been employed (Figure 2). A 99.99 percentile of 1,3-D air concentration of 60.3 ug/m^3 and 99.0 percentile of 15.5 ug/m^3 does not seem realistic. . It should not be assumed that concentrations in these ranges occur without measured concentrations in that range. The uncertainty in the measured air concentration probability distribution is evident from the width of the 95% confidence interval on the probability distribution. The lower 95% confidence interval values for this probability distribution are 9.3 ug/m^3 for the 99.99 percentile and 4.3 ug/m^3 for the 99.0 percentile. These air concentrations are in line with the modeled probability distribution (Figure 3). The 95% confidence intervals on the modeled concentration probability distribution are extremely narrow. This is because 5660 receptors comprise the input to fit that probability distribution. This is a very large input data set to characterize the distribution of air concentrations in the 9 township modeling domain so there is very little uncertainty in the shape of the distribution.

Figure 2. Probability plot of measured 1,3-D 14.5 month average air concentrations (ug/m^3).

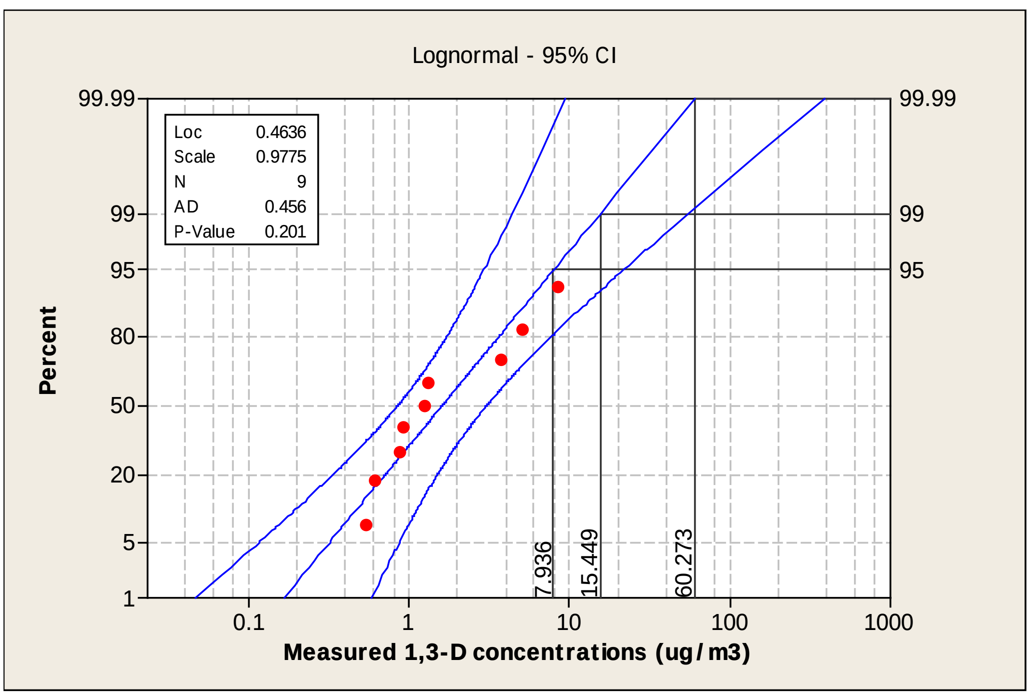


Figure 3. Probability plot of modeled 1,3-D 14.5 month average air concentrations(ug/m^3)..

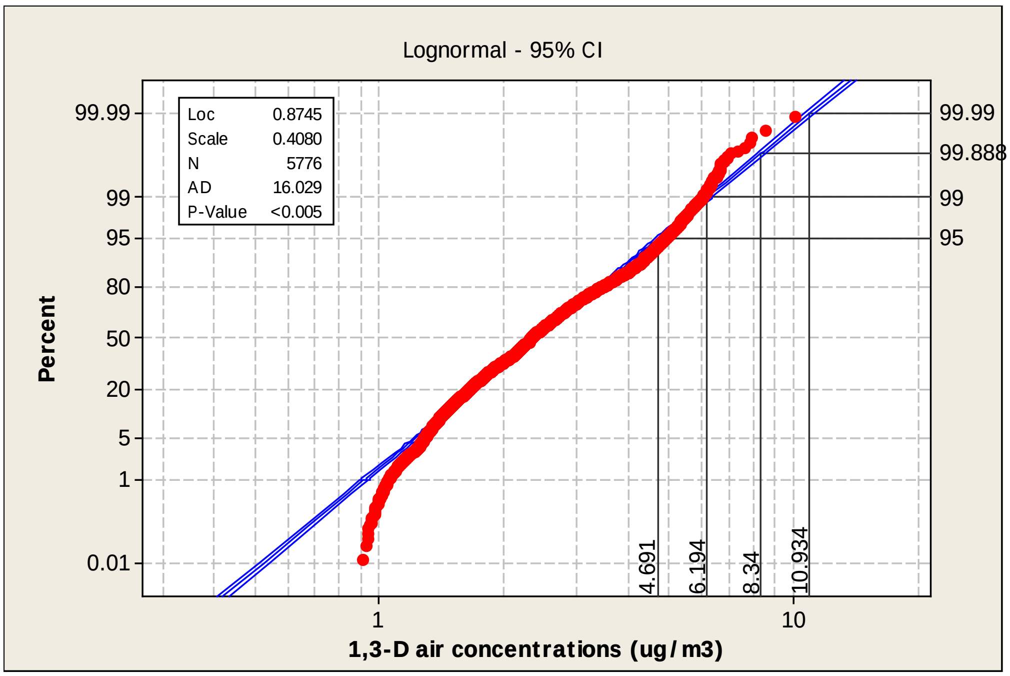
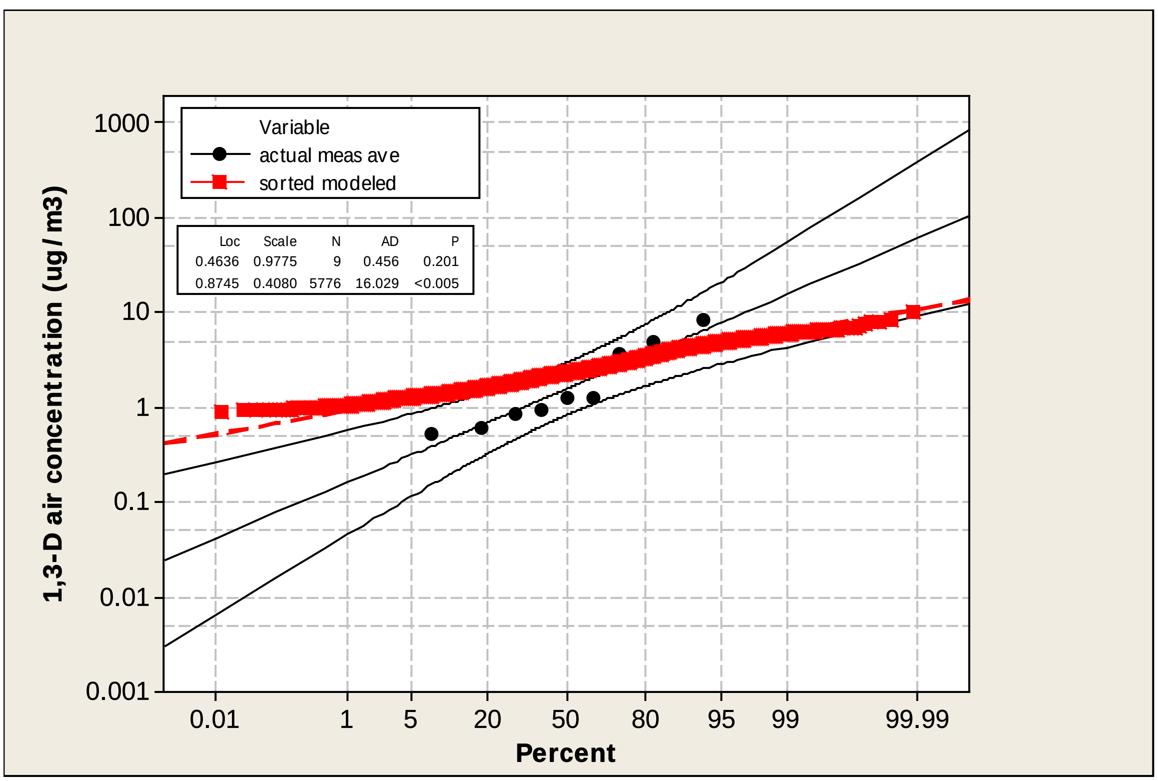


Figure 4 overlays the modeled 1,3-D air concentrations on the estimated measured 1,3-D air concentration probability distribution. The axes are transposed to make visual comparison between the two distributions easier. The same confidence intervals shown in Figures 2 and 3 are shown in Figure 4. Designating the measured values are the benchmark, the ISCST modeled air concentrations are significantly over estimated below the 50th percentile as illustrated by the many modeled values fall outside the measured air concentrations 95% confidence interval. This is consistent with the Dow findings. Above the 50% percentile the modeled values are lower than the measured values but all the modeled values fall within or at the lower 95% confidence interval on the measured air concentrations distribution. The match between these distributions will likely improve with new model runs after the errors in the stability class assignments and mixing height adjustments are corrected and the ISCST model is rerun using the validation scenario inputs with the corrected weather file.

Figure 4. Comparison of the estimated distribution of the measured 1,3-D air concentrations (ug/m^3) with estimated distribution of the SOFEA2 validation scenario modeled 1,3-D air concentrations (ug/m^3).



Conclusions:

The SOFEA2 model cannot be conclusively evaluated due to the following three factors:

1) The atmospheric stability classes assigned for many hours are in error.
2) The mixing height adjustment for many hours are in error.
3) The SOFEA2 model would not successfully perform the post processing of the ISCST modeled Merced validation scenario air concentrations. The SOFEA2 model bombed when attempting to conduct the post processing. As a result, none of the ISCST output files were closed and were lost.

All three of these factors must be fixed before DPR can move forward with a decision whether or not to use the SOFEA2 in house.

Preliminary analysis of the ISCST Merced validation scenario results indicates that if the three issues above are fixed the SOFEA2 model will likely produce modeled air concentrations that reflect the magnitude of the air concentrations measured by the 9 air samplers in the center of the 9 townships over the 14.5 month averaging period. The 72-hour and annual averages will be examined once the next version of SOFEA2 and the corrected Merced weather file with adjusted mixing heights are submitted.

The SOFEA2 model must run easily for scenarios other than those submitted by DOW and without any other significant issues before DPR can consider using it as a modeling tool.

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