Review Comments on the Report: Draft Air Dispersion Modeling of Methyl Bromide for Decision-Making Committee Produced by Todoroski Air Sciences, 2 November 2020

Sullivan Environmental Consulting, Inc.

1900 Elkin Street, Suite 200

Alexandria, VA 22308

14 November 2020

Contents

Executive Summary

Sullivan Environmental Consulting, Inc. (SEC) was requested by the Decision Making Committee (DMC) to review the Todoroski Air Sciences (TAS) modeling to identify errors and inconsistencies with DMC directives. This report documents our findings.

It should be noted at the outset that our review was based on the subset of files provided by TAS. We received 3,841 files from TAS without a "*readme*" document to explain how the modeling output was processed to produce the final concentration plots and buffer zone tables. Nevertheless, the transfer only provided detailed coverage for just 5 of the 23 scenarios that TAS had processed. The final TAS report that corrects the errors noted in this review should provide complete file transfer and a "*readme*" file and/or sufficient documentation in the report to allow others to replicate how the final plots and buffer zone tables were created.

The draft TAS modeling results do not provide reliable data to meet the DMC request. The following summarizes the most fundamental errors in the draft TAS document that SEC noted during our review based on the information made available:

1. **Source Treatments**: CALPUFF treats volume sources, such as the log stacks and ships, as virtual point sources. Without going into technical detail, the volume source treatment requires that the mid-point height of the source and the initial dilution along the vertical and horizontal axes be input to the model. The CALPUFF input files used by TAS as the basis for the modeling, on the other hand, used the full height of the log stacks and full height of the ships plus the portion of the holds below the water surface[1] as the effective height rather than the center point of the release. The TAS treatment centers the ship volume sources 20.1 m above the water surface rather than at the mid-point of the actual volume source, i.e. at 8 m above the water surface as documented in the Joint Expert Statements. A similar error was made by TAS for the log stacks. This effectively results in the sources being suspended above the port surface for the log stacks by approximately 2 m and the ships suspended above the water (by approximately 10 m).

[1] This includes the hold portion below water, which is not relevant to the airborne initial dispersion term. While the hold depth is approximately 20 m, much of the hold is below water and is not relevant to airborne modeling except to define the emission term.

Especially for the ship scenarios and the modeling within the port boundary, this unrealistic treatment produces anomalous results. We note that additional more minor discrepancies also occur in terms of how the initial conditions along the horizontal and vertical axes were specified.

2. **Time of Day**: Per the DMC directive, log stacks should have been vented between 7:00 AM and 7:00 PM and ships should have been vented starting at 10:00 PM onward (i.e. nighttime only for ships). Detailed files were only provided for Scenarios 1, 2, 3, 12, and 13 ("*scenario*-----.*dat*" CALRANK files from CALPOST). These files extracted the 9th highest annual 1-hour concentration at each receptor (99.9th percentile) and document the day and time the maximums occurred. The documented date/time for the 99.9th percentile concentrations for the various receptors show that for four of the five model output files, all hours of the day were used as the basis for extraction rather than maintaining log stack venting from 7:00 AM to 7:00 PM as required to be consistent with the DMC directives. Ship venting that should have been at night was adversely affected by the same problem. Considering the marked differences in dilution conditions on a daytime and nighttime basis, this erroneous treatment introduces substantial model bias for the ship and log stack scenarios, with the exception of Scenario 2, which limited the log stack only assessment properly to within the 7:00 AM to 7:00 PM as directed. Our review showed the following timing sequences used in these scenarios in Table E-1:

Table E-1: Timing of TAS Venting Assumptions for Available Scenarios

Scenario #	Description	Time of Day Modeled
1	Worst case logs & ships	All hours
2	Worst case logs only	7:00 AM to 7:00 PM
3	Worst case ship only	All hours
12	Logs buffer worst case, 3 log stacks	All hours
13	Logs buffer worst case, 1 log stack	All hours

The 99.9th percentiles based on all hours of the day as determined by TAS are not relevant to the matter at hand.

3. **Receptor Resolution**: The Expert Joint Statements provide very detailed specifications for a fine grid spacing within the port to ensure that modeling results would capture the fine scale impacts near sources. TAS has not complied with this directive and on this basis did not comply with the DMC directives. While the fine spacing directed requires extensive run times, this is needed to comply with the DMC directive and the Joint Expert Statement. The spacing relied on in the TAS report was much more coarsely spaced, which would be expected to miss actual peak values. For example, within the port boundary the grid spacing had up to four times fewer receptor locations in the model than required.

4. **Statistical Treatment of 99.9th Percentile:** It is unclear how the 99.9th percentile plots and buffer zones were computed. Based on the runs available for review (Scenarios 1, 2, 3, 12, and 13) there are three years that were separately processed with the 9th highest values (99.9th percentile on an annual basis) selected. It is unclear if the maximum 99.9th percentile concentrations over the three-year period were used or the average 99.9th over the three years was used as the basis for the plots and buffer zones. There is not any documentation in the report or available files that explains the basis for the concentration plots. We also did not see the actual plot files in the data provided.

   When three years of meteorological data are modeled and the goal is to compute the 99.9th percentile, as directed by the DMC, then the full three years should have been the basis for selecting the 26th highest value within the full distribution at each of the receptors, which would be the actual 99.9th percentile for the three-year period. Other approaches would not be statistically correct.

In summary, the draft TAS modeling does not comply with the DMC directive and the Joint Expert Statement.

1.0 Overview

The Decision Making Committee (DMC) has requested that Sullivan Environmental Consulting, Inc. (SEC) review the draft report produced by Todoroski Air Sciences (TAS) on 2 November 2020 entitled: *Draft Air Dispersion Modeling of Methyl Bromide for Decision-Making Committee.*

The following summarizes the relevant paragraphs from the DMC directions on the 28th August 2020 and the 28th of September 2020. SEC has followed these directives and have limited our comments at this time only to errors in the modeling and areas where the DMC directives have not been followed.

- **Paragraph 6**: The DMC requests that modelling should occur using the parameters, model choices, and inputs agreed to in the joint statements reporting on the expert conferencing, and used in the June 2020 SEC modelling, unless superseded by other information in this Direction and Minute. *(Direction & Minute WGT023 of the Decision-making Committee (DMC) – 28 August 2020).*

- **Paragraph 8***:* The DMC notes that an independent review of the modelling is required to confirm that that there are no errors in the set up and performance of the models. *(Direction & Minute WGT023 of the Decision-making Committee (DMC) – 28 August 2020).*

- **Paragraph 10d**: The independent expert is to review the TAS modelling for the purpose of confirming that the models have been created and performed correctly in line with the expert conference joint statements and this Direction and Minute. *(Direction & Minute WGT023 of the Decision-making Committee (DMC) – 28 August 2020).*

- **Paragraph 11**: The DMC considers that SEC and Atmospheric Sciences Global (ASG) are appropriate expert parties to review the modelling. The DMC considers that TAS's

pre-modelling liaison with SEC and ASG should be restricted to just the assumptions behind those parameter values that differ from the expert conferencing. *(Direction & Minute WGT024 of the Decision-making Committee (DMC) – 28 September 2020).*

- **Paragraph 15**: The DMC would like to clarify that this review shall be limited to reviewing errors in the modelling itself, for example identifying if inaccuracies are introduced due to errors in the modelling program, output processing or other issues with the operation of modelling or processing of data. *(Direction & Minute WGT024 of the Decision-making Committee (DMC) – 28 September 2020).*

- **Paragraph 16**: The DMC emphasizes that it is not requesting a review of the selection of modelling protocol, processing procedure, or the assessment and conclusions of the modelling output, except where a decision by the modeller results in a fundamental error. *(Direction & Minute WGT024 of the Decision-making Committee (DMC) – 28 September 2020).*

- **Paragraph 17**: The DMC considers that there has been sufficient information and discussion regarding the operation and processing of modelling in the material already shared with the DMC during the submission period, expert conferencing, and the hearing. As such, further discussion and analysis of these matters is not required. *(Direction & Minute WGT024 of the Decision-making Committee (DMC) – 28 September 2020).*

2.0 Emission Treatments

Although TAS used a different number, orientation and set of log rows for most scenarios, the emission rates on a comparable volume basis were similar to the Joint Signed Statement and the values used by SEC. Some relatively small differences were found. The ship holds also generally matched the values determined by SEC.

The approach followed the agreement set by the Joint Signed Statement to assume 50% desorption of the log rows during the first hour, followed by 1% for each hour during the next 12 hours for log rows. For the ships, TAS followed the approach of assuming emissions based on 17.5 + 3% desorption =20.5% of the log sorption rate for the first hour for the ship holds, followed by 18.5% for the second hour, and then over the next 11 hours releasing approximately 1 % per hour is desorbed for the ship holds. This approximately matches the expert statement although there is an extra hour of emissions at the 13th hour.

It is noted that the TAS emission rate of 2.1 g/sec was based on 0% capture efficiency rather than 30% capture efficiency as indicated in the spreadsheet. In addition, the last emission rate carries the error and creates a larger emission rate than the uncontrolled emission rate for Scenario #15 as shown in Table 2-1.

We agree with the ship hold emissions calculations provide by TAS in Table 2-2.

Table 2-1: Comparison of TAS Log Row Emission Rates with SEC Comparable Emission Rates

SCN	Log Treatments Rate g/m3	Log Row Recapture %	TAS Emissions (g/sec)	SEC Emissions (g/sec)	Fraction of Logs with Recapture % *** Applied to log stacks, ships 100% always**	Confirmation
1	120	30%	2.10	1.89	50%	Log Recapture 0% not 30%
2	120	30%	2.10	1.89	50%	Log Recapture 0% not 30%
3	-	-	-		-	-
4	72	30%	1.26	1.13	50%	Log Recapture 0% not 30%
5	72	30%	1.26	1.13	50%	Log Recapture 0% not 30%
6a	-	-	-	-	-	-
6b	-	-	-	-	-	-
7a	72	60%	0.72	NA	50%	Files Not Available for Review
7b	72	60%	0.72	NA	50%	Files Not Available for Review
8	72	60%	0.72	NA	50%	Files Not Available for Review
9	-	-	-	-	-	-
10a	72	60%	1.08	NA	75%	Files Not Available for Review
10b	120	90%	0.60	NA	100%	Files Not Available for Review
10c	72	90%	0.36	NA	100%	Files Not Available for Review
10d	40	90%	0.20	NA	100%	Files Not Available for Review
11a	72	60%	1.08	NA	75%	Files Not Available for Review
11b	120	90%	0.60	NA	100%	Files Not Available for Review
11c	72	90%	0.36	NA	100%	Files Not Available for Review
11d	40	90%	0.20	NA	100%	Files Not Available for Review
12	120	30%	2.10	1.89	50%	Log Recapture 0% not 30%
13	120	30%	2.10	1.89	50%	Log Recapture 0% not 30%
14	-	-	-	-	-	-
15	120	0%	3.00	2.08	50%	Emissions Higher for Log Recapture of 0%

Table 2-2: Comparison of TAS Ship Hold Emission Rates with SEC Comparable Emission Rates

SCN	Ship Treatment Rate g/m3	Ship Hold Recapture %	TAS Emissions (g/sec)	SEC Emissions (g/sec)	Confirmation	
1	120	0%	324.28	324.14	√	
2	-	-	-	-	-	
3	120	0%	324.28	324.14	√	
4	72	0%	194.57	194.49	√	
5	-	-	-	-	-	
6a	72	0%	194.57	194.49	√	
6b	72	50%	97.28	97.24	√	
7a	72	0%	194.57	NA	Files Not Available for Review	
7b	72	50%	97.28	NA	Files Not Available for Review	
8	-	-	-	-	-	
9	72	0%	194.57	NA	Files Not Available for Review	
10a	72	0%	194.57	NA	Files Not Available for Review	
10b	120	50%	162.14	NA	Files Not Available for Review	
10c	72	50%	97.28	NA	Files Not Available for Review	
10d	40	50%	54.05	NA	Files Not Available for Review	
11a	-	-	-	-	-	
11b	-	-	-	-	-	
11c	-	-	-	-	-	
11d	-	-	-	-	-	
12	-	-	-	-	-	
13	-	-	-	-	-	
14	40	0%	108.09	108.05	√	
15	-	-		-	-	

Deviations from Signed Joint Statement and Other Errors Noted for Emission Treatments

1. For four of the five output files provided, TAS has modelled log stacks and ship hold emissions for most scenarios venting any hour of the day instead of daytime operations for log stacks and nighttime hours as for ships. When doing hypothetical combined ships and logs assuming daytime ship venting is appropriate as a hypothetical analysis, although such overlap is not planned for actual port operations. TAS should have modeled ship emissions at least for ships as nighttime venting: "*Modelling assuming opening the five holds at two-hourly intervals starting at 10pm, 12am, 2am, 4am, and 6am."* Since this was not done, the ships only analyses do not realistically represent port operational practices. Similarly, venting log stacks all hours of the day (as was found in all but one of the five example outputs provided) deviates from the DMC directive and does not represent actual port operations.

2. There were typographical errors in the equation using recapture percentage. In both cases in this equation the "%" needs to be divided by 100 to correctly show the remaining fractions.

   *Emission rate (g/s) = (Initial Dose (g/m^3)) x (1-Recapture(%)/**100**) x (Volume of log stacks under sheet enclosure or in ship holds (m^3)) x (Percentage (%)/**100** of recapture applied to log stacks under sheet enclosure or in ship holds) / 3600 (seconds).*

3. The report states that the ship hold emissions followed a pattern of 10 additional hours of 1% loss rate after the first 2 hours; however, the CALPUFF VOLEMARB ship hold emissions files show that an additional hour was added making it 11 hours of 1% loss rate by desorption.

3.0 Source Characteristics for Log Stacks and Ships

TAS used source characteristics in the modeling files that were inconsistent with the Signed Joint Statement of January 30th, 2020 and standard modeling practice. The observed deviations are summarized below.

- The effective source heights were listed as 3 m for the log stacks and 8 m above sea level for ships in the Signed Joint Statement. TAS did not follow this direction. Rather, the values used by TAS as documented in the VOLEMARB files were 5 meters for the log rows (not 3 m) and 20.1 meters for the ship holds (not 8 m). The CALPUFF model uses a virtual point source method to represent volume sources where the effective height of the source is set to the center point of the volume source. As stated in the CALPUFF user's guide, the effective height of a volume sources is "*the effective height (m) above the ground (*in this case water surface*) of the puff center*." The approach used by TAS, on the other hand, set the effective height of the volume sources associated with ships for example, at 20.1 above the water surface rather than at 8 m as specified in the expert statements. TAS then used the initial vertical dimension (SIGMA zo) as 4.67 m. Since the volume source vertical dimensions are defined as 2.15 heights above and below an elevated volume source like this, the modeled source including initial conditions is 10 m to 30 m above the water surface. In other words, in the TAS model treatment, the ship is suspended ~ 10 m above the water. All near-field impacts within the port boundary are adversely affected by this error. The isopleth analyses and buffer zone assessments are unreliable. A similar error in defining the effective height of the volume source as the top of the source also affected the log stacks, although the error was not as large. Refer to Table 3-1 for details.

- The Sigma Y values should have been set to the diagonal length as agreed to in the Signed Joint Statement. The basis for the TAS calculations were not provided and therefore, were not able to be replicated. The values used, however, are inconsistent with the Expert Statement.

- The Sigma Z values were not correct.

- The log rows width was set up as 6 meters plus an additional 1-meter buffer zones between rows instead of 5 meters for each row source with an additional buffer between the log rows of 1 meter. The height of the log rows was set to 5 m instead of 6 m as agreed in the Joint Signed Statement.

Table 3-1: Source Specifications for the Log Stack and Ship Sources[2]

Parameter	TAS Value (m)	Signed Joint Statement (m)	Notes
Length of Log Row	6	-	-
Width of Log Row	6	-	-
Effective Height of Log Row	5	3	Effective Height should be 6/2=3 m
Separation between Rows	1	-	-
Sigma Y	2.33	1.97	Should be Diagonal Length/4.3
Sigma Z	1.16	1.40	Should be Height/2.15
Length of Ship Hold	22	30	22 m Ship Hold Length is ok
Width of Ship Hold	22	30	22 m Ship Hold Width is ok
Height of Ship Hold	20.1	8	Effective Height should be 8 m
Separation between Holds	Variable	-	-
Sigma Y	5.12	6.33	Should be Diagonal Length/4.3
Sigma Z	4.67	3.72	Should be Height/2.15

[2] Standard practice for modeling initial conditions for a volume source is to set the horizontal component based on the length of the side divided by 4.3; however, we agreed to use the diagonal of the face of the log row pile to substitute the Length as agreed in the Signed Joint Statement. Similarly, the initial vertical conditions are set to the height of the source above ground level (or in the case of a ship the freeboard height above the water surface) is divided by 2.15.

4.0 Modeling Files and File Processing

Within the allocated time constraints, SEC reviewed the modeling files provided by TAS. While 3,841 files were transferred to SEC they were sent without a "*readme*" document or sufficient documentation in the report to explain how TAS arrived at the final isopleth maps and buffer zone tables. Furthermore, despite the large number of files, percentile results for only five of the 23 scenarios were provided. In order for this process to be transparent and allow for sufficient replication by the applicant and other interested parties, TAS needs to provide all files and provide sufficient documentation regarding how the results were processed into the final figures and buffer zone table. Besides missing post-files for 18 of the 23 model scenarios, the final processed plot files used by TAS to create the isopleth analyses in the report and appendices also need to be provided for all model scenarios in order to support a more thorough review. The final report should have full coverage of the modeling files and sufficient documentation of how the final results were processed. The following briefly summarizes the review of the modeling files that could be accomplished based on the limited information provided:

- A review of all the CALPUFF model options used in the TAS modeling and verified that they used the same options SEC.

- It was verified that all 432 model files for the log sets were correctly set up (6 log sets, 3 years, 24 hours), except for other comments in this document where errors and deviations are specifically noted.

- It was verified that the 72 model files for the ship containers were correctly set up (1 ship, 3 years, 24 hours), except for other comments in this document where errors and deviations are specifically noted.

- It was verified that the modeled sources parameters (VOLEMARB files) matched the Table 3-1 source summary in the Todoroski report.

- It was verified that the source emissions, as described on Page 5 of the Todoroski report matched the emissions in the VOLEMARB files with one exception. Where TAS mentions that the ship emissions during the first hour is 21%, the second hour is 18% and that the remaining 10 hours are 1% of the initial dose, they modeled with 11 hours of 1% emissions.

- Table 4-1 provides a comparison of the varying grid resolutions defined by the model protocol versus the TAS modeling. As noted below, TAS relied on a coarser grid than

specified in the Joint Signed statement within the port boundary, and did not provide the required 20 m spacing along the port boundary as specified in the Joint Signed Statement. It would be expected on this basis that the actual maximum concentrations are missed within the coarser receptor set used by TAS.

Table 4-1: Comparison of Model Grid Resolution

DISTANCE FROM CENTER	MODEL PROTOCOL	TAS MODELING
OUT TO PORT BOUNDARY	25 m	
UP TO 60 m		12-13 m
60 m-180 m		25 m
FENCELINE	20 m	
180 m TO 0.75 km		50 m
FENCELINE TO 1 km	50 m	
0.75 m to 1.5 km		100 m
1 km TO 3 km	100 m	
1.5 km to 3 km		

- The basis for the isopleth maps in Appendices A and B and the buffer zone table (Table 4-1 in the TAS report) is not specified in the TAS report or provided files. The plot files needed to replicate this work and verify model processing were not provided for any scenarios. The CALPOST CALRANK output files (e.g. scenario..1…..date) that were used to identify the 99.9th percentile (9th highest value for each receptor) for each year were only provided for five of the scenarios (Scenarios 1 ,2, 3,12, and 13). TAS extracted the 9th high (99.9th percentile) separately for each of three years, but it is unclear what is being plotted and what is used to compute buffer zones. The actual plot files used to create the figures in Appendix A of the TAS report, and the basis for the buffer zone table was not found within the data provided.

Statistically, the correct way to compute the 99.9th percentile of a three-year data set would be to merge the three years and extract the 26th high value for each receptor. No basis was provided to confirm this was done. It also is unclear if TAS used the maximum 99.9th percentile within the three separate years that were run or used the average 99.9th percentile across the three years as the basis for the isopleth plots and buffer zones. Such details need to be clearly described in the final report for the results to be interpreted.

- All isolines on the contour maps should be labelled or color coded so the concentrations can be determined.

- A review of the model scenario files provided (only for scenarios 1, 2, 3, 12, and 13) determined that model Scenario 2 determined the 9th highest concentrations for each receptor were based on the daytime hours of 7:00 AM to 7:00 PM. The 9th highest concentrations for other four model scenarios were incorrectly based on assuming venting occurred on all hours of the day.

5.0 Review Relative to Measured Data

Per Paragraph 17 of the 30 January 2020 Joint Statement of the Expert Panel, "*Use monitoring data to inform performance of model, is needed for far-field analysis.* " The TAS modeling included far-field analysis. Per the signed joint statement such review should be performed by TAS to ensure that the modeling is sufficiently realistic to support regulatory decisions. There are no such comparisons in the TAS report.

6.0 Conclusions

Review of the draft TAS modeling report, which was directed by the DMC, has indicated that corrections are needed in multiple areas as specified in this report to comply with the directives of the DMC and to produce error-free modeling results. To support review of the final modeling, which presumably will address the deficiencies noted in this and other reviews, full documentation will be needed rather than providing files with limited coverage. This will allow for a more thorough review based on the availability of all modeling files and an explanation of how TAS processed the modeling output to compute the 99.9th percentile values shown in isopleth analyses and buffer zone tables.