U-ESS-Z-00001
Revision 0
May 2015

Evaluation of the Safety of the Situation (ESS): Higher than Expected Concentration of Methyl Mercury in Tank 50 (PISA PI-2015-0007)

APPROVALS

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1.0 PISA Description/Summary

Potential Inadequacy in the Safety Analysis (PISA) PI-2015-0007 pertains to the Saltstone Facility Documented Safety Analysis (DSA), WSRC-SA-2003-00001, and is described in the PISA Database as follows:

"The Saltstone permit requires that Toxic Characteristic Leaching Procedure (TCLP) be performed quarterly. This is accomplished via samples obtained from Tank 50. The fourth quarter 2014 Tank 50 sample did not pass the TCLP. Part of the investigation into why this occurred involved mercury speciation analysis on the fourth quarter Tank 50 sample as well as the first quarter 2015 Tank 50 sample. Sample results received on 4/1/15 indicate that the concentration of methyl mercury (monomethyl mercury or MMHg) in Tank 50 (53.5 mg/L not accounting for analytical uncertainty) exceeds the bounding concentration assumed in the Saltstone safety basis (1.1 mg/L). On 4/2/15, Facility Management determined that this discovery of a larger than expected organic constituent of mercury in the system be reported as a management concern to share information with the complex. Therefore, an Occurrence Report was generated (EM-SR-SRR-LWOGEN-2015-0001) that placed the Tank 50 to Saltstone transfer procedure on Administrative Hold until an evaluation was completed characterizing the impact of elevated MMHg on Saltstone DSA assumptions. Prior to that time (2/3/15), approximately 54kgal of the high MMHg material was processed through the Saltstone facility and placed into SDU Vault 5B.

The review of the Saltstone DSA assumptions identified five accident scenarios that exceed the PAC-3 threshold value at a MMHg concentration in the Salt Waste Feed of 95.2 mg/L (2 sigma uncertainty applied to the analysis result of 53.5 mg/L). Three of the accidents involve salt solution waste in the Saltstone vault drainwater systems, and two of the accidents involve NPH events around salt solution waste transfers into the Salt Feed Tank (SFT).

Additionally, the SFT explosion accident scenario, while not exceeding the PAC-3 threshold for MMHg, would constitute a decrease in the overall margin of safety. Table 3.6-7 of the Saltstone DSA denotes key hazardous chemicals in salt solution as a Y (yes) in the table. This is based on whether the chemicals contribute greater than or equal to 25% of their individual PAC-3 threshold values corresponding to the source term created by a Salt Feed Tank (SFT) explosion. None of the chemicals in the table exceed the PAC-3 threshold (limiting chemical is aluminate at ~59% of PAC-3). The current safety basis concentration of methyl mercury (CH_3Hg, 1.1 mg/L) as listed in DSA Table 3.6-7 contributes less than 25% of its PAC-3 and is not considered a "key hazardous chemical in salt solution". At 95.2 mg/L (2 sigma on reported sample result of 53.5 mg/L), methyl mercury exceeds 25% of PAC-3 and becomes the new limiting contributor (i.e., ~ 90% of PAC-3 versus ~59% of PAC-3 from Aluminate) associated with a SFT explosion."

Additional information pertaining to PISA PI-2015-0007 includes:

- Date of Discovery: 04/10/2015
- ORPS Report Number: EM-SR--SRR-WSALT-2015-0001

References pertaining to PISA PI-2015-0007 and this Evaluation of the Safety of the Situation (ESS) include:

1. Saltstone Facility Documented Safety Analysis. WSRC-SA-2003-00001, Rev. 11, July 2014.
2. "Results of Preliminary Hg Speciation Testing on 4Q14 Tank 50, 1Q15 Tank 50, and SRNL 14-Day TCLP Leachate", SRNL-L3100-2015-00054, Rev. 0, April 2015.
3. Saltstone Chemical Evaluation (U). S-CLC-Z-00034, Rev. 8, August 2010.
4. Consolidated Hazard Analysis for Saltstone Disposal Units 3 and 5 Project. S-CHA-Z-00004, Rev. 0, February 2013.
5. Consolidated Hazard Analysis for Modifications to the Saltstone Facility Process Room in Support of the Enhanced Low Activity Waste Disposal (ELAWD) Project. S-CHA-Z-00003, Rev. 0, September 2011.
6. Volatilization and Flammability Characteristics of Elemental and Organic Mercury. X-ESR-G-00048, Rev. 1, May 2015.
7. Saltstone Facility Consolidated Hazard Analysis (U). WSRC-TR-2001-00574, Rev. 15, April 2014.
8. Maximum Source Terms for Staying within Chemical PAC Limits (U). S-CLC-Z-00088, Rev. 2, September 2011.
9. Maximum Source Terms for Staying within Chemical PAC Limits (U). S-CLC-Z-00088, Rev. 3, November 2012.
10. "Kinetic Treatment of Dimethyl Mercury Degradation and Formation Studies", SRNL-WHM-2004-00006, Rev. 0, September 2004.
11. Waste Acceptance Criteria for Aqueous Waste Sent to the Z-Area Saltstone Production Facility (U). X-SD-Z-00001, Rev. 13, January 2014.
12. "IH Baseline Monitoring for Combustible Atmosphere for SDU 4", SRR-FSH-2014-00003, May 15, 2014.
13. "Saltstone Facility Air Monitoring Results 251-4Z (Vault 4) Cell E", SRR-WTF-2015-0001, February 11, 2015.
14. "Saltstone Facility Air Monitoring Results for Salt Disposal Units 2A and 2B", SRR-WTF-2015-00002, February 11, 2015.
15. "Saltstone Facility Air Monitoring Results 251-4Z (Vault 4) Cell F", SRR-WTF-2015-00004, May 13, 2015.

16. "Saltstone Facility Air Monitoring Results 251-4Z (Vault 4) Cells E and J", SRR-WTF-2014-00011, August 12, 2014.

17. "Saltstone Facility Air Monitoring Results 251-4Z (Vault 4) Cell K", SRR-WTF-2014-00015, September 16, 2014.

18. "Saltstone Facility Air Monitoring Results 251-4Z (Vault 4) Cell L", SRR-WTF-2014-00016, September 16, 2014.

19. "Saltstone Facility Air Monitoring Results 251-4Z (Vault 4) Cell D", SRR-WTF-2014-00017, September 16, 2014.

20. Saltstone Facility Consolidated Hazards Analysis (CHAP) Basis (U). S-CLC-Z-00035, Rev. 3, October 2010.

21. Technical Safety Requirements, Saltstone Facility. S-TSR-Z-00002, Rev. 13, November 2014.

22. Fire Hazards Analysis for Saltstone Disposal Facility. F-FHA-Z-00003, Rev. 1, August 2013

23. Proposed Chemical Compounds and Concentration Limits for Saltstone Salt Solution. X-CLC-Z-00033, Rev. 3, September 2012.

2.0 Compensatory Measures / Operational Restrictions

2.1 PISA Compensatory Measures / Operational Restrictions

The following compensatory measures are currently in place as documented in PISA PI-2015-0007:

2.1.1 Transfers of material containing monomethyl mercury into or out of the Saltstone Salt Feed Tank are prohibited.

2.1.2 Transfers of material containing monomethyl mercury out of the Saltstone Disposal Units (SDUs) or Vault 4 are prohibited.

2.2 ESS Compensatory Measures / Operational Restrictions

The evaluation provided in this ESS demonstrates that the concentration of MMHg within the Saltstone Safety Basis (SB) can be significantly increased above the current value of 1.1 mg/L. The concentration of MMHg could be increased to a point at which it will be limited by the concentration of total mercury currently permitted into the facility (358 mg/L DSA value which is further limited to 325 mg/L in Reference 11).

Additionally, in preparation of the ESS (see Section 3.2), it was recognized that a potential formation/production rate of dimethyl mercury (DMHg) exists given the presence of mercury (II) and organics (Ref. 10). Reference 6 demonstrates that DMHg is flammable, which the SB does not currently recognize. Therefore, Attachment B was created to form the basis for the compensatory measure provided below. The compensatory measure provided below works in conjunction with Limiting Condition of Operation (LCO) 3.1.3 of the Saltstone Technical

Safety Requirements (TSR, Ref. 21) and is the only compensatory measure required for PISA PI-2015-0007.

- The cell GROUT height in SDU 3 (Cells A and B) and SDU 5 (Cells A and B) shall be less than or equal to 19.0 feet (accounts for the same 0.25 foot uncertainty as applied from Reference 21). All Required Actions and Completion Times of LCO 3.1.3 remain applicable, including their bases.

As a result of the above compensatory measure, Surveillance Requirements (SRs) 4.1.3.1 and 4.1.3.2 shall be adjusted accordingly (i.e., 21.5 feet becomes 19.0 feet for both SRs and 20.5 feet becomes 18.0 feet for SR 4.1.3.2). All SR frequencies and bases remain applicable.

3.0 Safety Assessment Results

3.1 Immediate Safety Assessment

The review of the Saltstone SB, including supporting documents, identified five accident scenarios that exceed the Protective Action Criteria (PAC)-3 threshold value with a MMHg concentration in the Salt Waste Feed of 95.2 mg/L (2 sigma uncertainty applied to the analysis result of 53.5 mg/L). From Reference 4, three of the accidents involve salt solution waste in the Saltstone drainwater systems (NODE10C-1-001, NODE11-6-0016, NODE11-6-0017), and two of the accidents (NODE11-7-0021, NODE11-7-0026) involve Natural Phenomena Hazard (NPH) events around salt solution waste transfers into the Salt Feed Tank (SFT). All of the aforementioned events deal with significant quantities of material at risk being heated due to various initiating events. The associated analyses (Ref. 5 and 8) treat MMHg as a volatile chemical. As such, the accident source term is set equal to the material at risk. The gallons of source term required to exceed the PAC-3 threshold is proportional to the concentration. At 95.2 mg/L, the concentration is approximately 86 times that assumed in the existing DSA (95.2 mg/L / 1.1 mg/L). At 1.1 mg/L, the gallons to exceed PAC-3 for MMHg is 77,100gallons (Ref. 9). Decreasing this value 86 times results in approximately 890 gallons of source term to exceed PAC-3. All of the events previously discussed exceed 890 gallons.

The SFT explosion accident scenario, while not exceeding the PAC-3 threshold for MMHg, would constitute a decrease in the overall margin of safety. The SFT explosion is based on a stoichiometric Isopar L explosion with a source term (for volatiles) of 7513 gallons (Ref. 3). At 1.1 mg/L, the source term to exceed the PAC-3 threshold (50% meteorology [met] and 100 cm surface roughness[SR]) is 712,000 (Ref. 9). Therefore, the current percentage of PAC-3 for MMHg is approximately 1 percent (7513 gal / 712,000 gallons X 100). Increasing this percentage by a factor of 86 does not reach 100 percent of the PAC-3 threshold.

In addition, Table 3.6-7 of the Saltstone DSA denotes key hazardous chemicals in salt solution as a Y (yes) in the table (Ref. 1). This is based on whether the chemicals contribute greater than or equal to 25% of their individual PAC-3 threshold values

corresponding to the source term created by a SFT explosion. None of the chemicals in DSA Table 3.6-7 exceed the PAC-3 threshold (limiting chemical is aluminate at ~59% of PAC-3 as shown in Reference 3). As shown previously, the current SB concentration of methyl mercury (1.1 mg/L as listed in DSA Table 3.6-7) contributes less than 25% of the PAC-3threshold and is not considered a key hazardous chemical in salt solution. At 95.2 mg/L (2 sigma on reported sample result of 53.5 mg/L), MMHg exceeds 25% of PAC-3 and becomes the new limiting contributor (i.e., ~ 86% of PAC-3 versus ~59% of PAC-3 from Aluminate) associated with a SFT explosion. This would require the MMHg to be added to the Waste Acceptance Criteria (WAC) as a key hazardous chemical (i.e., included in the Tank 50 sample analysis).

An Unreviewed Safety Question Evaluation (USQE), USQ-SS-2015-00083, was performed for PISA PI-2015-0007 and resulted in a "positive" evaluation. As part of the initial safety assessment, the USQE was performed against the existing SB that analytically treats MMHg as a volatile chemical. The USQE was "positive" based on a "yes" answer to the following questions:

Question 2 - "…increase the consequences of an accident previously evaluated in the Safety Basis?" (At the increased MMHg concentration, several hazards analysis events now exceed the chemical consequence criteria using the Code of Record PAC-3 threshold for MMHg) and,

Question 7 - "…decrease the margin of safety?" (The increase in MMHg concentration is such that the 25% threshold documented within the DSA WAC Specific Administrative Control would be exceeded).

With the Compensatory Measures identified in the PISA (repeated in Section 2.1 above) and Section 2.2 above, the facility is in a safe condition as the events of concern are precluded. Section 3.2 provides the final safety assessment that allows removal of the Compensatory Measures of Section 2.1.

3.2 Final Safety Assessment

Reference 6 documents the mostly likely form of mercury (Hg) in the waste stream based on the salt solution composition, literature searches, and testing performed by Eurofins Frontier Global Sciences, Inc. The testing demonstrated the majority of Hg is in the form of MMHg, with relatively smaller amounts of elemental, ionic, ethyl, and dimethyl mercury (DMHg). Per Reference 6, the likely MMHg compounds in the liquid waste stream are not volatile due to low vapor pressures, low Henry's Law coefficients, and water solubility. In addition, the lowest melting point of all the methyl mercuric species is shown to be ≥ 100°C and can be treated in accident analysis as a solid (Ref. 6). MMHg has the lowest PAC-3 threshold value (2.15 mg/m^3) for the Hg compounds listed in Revision 26 of the database, which is the code of record revision for the Saltstone Facility. Some of the aforementioned species have no documented PAC-3 threshold value in Revision 26 of the database (e.g. ethyl mercury). From a chemical consequence perspective, these can be considered bounded by the MMHg

evaluation provided in this ESS. An evaluation of the Saltstone SB and supporting documents (Ref. 4, 5, and 7) has shown that the allowable MMHg concentration to remain below the PAC-3 threshold is significantly greater than the current total mercury concentration in the Saltstone WAC (limit of 325 mg/L from a DSA safety analysis value of 358 mg/L) when the MMHg is treated as a non-volatile solid versus a volatile (see Attachment A).

Attachment A illustrates the allowable MMHg concentration to remain below the PAC-3 threshold. To determine the percentage of PAC-3 threshold, aligning with current DSA bounding event scenario (SFT Explosion), the following evaluation is provided.

Using the original source terms for the MMHg compounds to exceed the PAC-3 threshold values from Reference 9 (712,000 gallons utilizing 50% met and 100 cm SR and 77,100 gallons utilizing 95% met and 3 cm SR), the updated source terms (treating MMHg as a solid) will be calculated by ratioing to the new concentration of 358 mg/L (DSA mercury concentration from Reference 1, Table 3.6-7).

Reference 9 criteria:

The chemical is “solid” if its melting point is >100°C
The chemical is “liquid” if its melting point is <100°C but its boiling point is >100°C
The chemical is “volatile” if both its melting point and boiling point are <100°C.

Converting mercury to MMHg concentration:

358 mg/L / 200.59 g/mole X 215.63 g/mole = 384.8 mg/L

Determining gallons to exceed PAC-3 threshold:

712,000 gal X 1.1 mg/L / 384.8 mg /L = 2035 gal (NPH rollup events or code of record for application of meteorology)

77,100 gal X 1.1 mg/L / 384.8 mg/L = 220 gal (individual and NPH Events)

Thus, in evaluating the consequences associated with MMHg, it is treated as a solid and is not considered to be entirely released if heat is applied (i.e., SFT explosion) or partially released based on the heat available to bring the chemical to it boiling point (methodology used in References 4, 5, and 7). The bounding source term from the Saltstone accident analysis for solids (or precipitates) is the SFT explosion which has a source term of 7.64 gallons (Ref. 3). Thus, the MMHg percentage of PAC-3 is 7.64 gal / 2035 gal X 100 = 0.38%. Therefore, consistent with Table 3.6-7 of Reference 1, MMHg would not need to be considered a key hazardous chemical.

By allowing the MMHg concentration to be set equal to the total mercury DSA concentration (i.e., approximately 358 times greater than current concentration) raises the question of whether this provides a source for producing significant DMHg.

Reference 10 establishes that the kinetics of the first methylation are fast compared to the second. Therefore, the incoming distribution of mercury between Mercury (II) and MMHg does not affect the DMHg formation/production rate.

However, it was recognized that the formation/production rate of DMHg that currently exists is not recognized in the Saltstone SB. This, in conjunction with Reference 6 which demonstrates that DMHg is flammable, drove the need to assess the flammability impacts to the SDUs and SFT. Reference 6 further documents that the DMHg contribution to the lower flammability limit bounds all other dialkyl species (diethyl, dipropyl, dibutyl). Attachment B documents this assessment and establishes the basis for the compensatory measure in Section 2.2. The assessment for SDUs 3 and 5 includes the aforementioned DMHg formation/production rate from Reference 10 (applied to the DSA value of 358 mg/L for total mercury and adjusted to address the diethyl, dipropyl, and dibutyl) as well as the inventory permitted by Reference 11 (1.1 mg/L DMHg). Attachment B assumes an SDU temperature of 81°C, which is the highest temperature evaluated in Reference 10 for a DMHg rate constant in salt soltution. A review of temperature data for SDU 2 (Cells A and B) from the PI database illustrates that the peak temperature did not exceed 68°C. Additionally, Reference 22 documents that the grout, under normal circumstances, does not exceed an average temperature of 75°C. Therefore, utilizing an average bulk temperature of 81°C for SDUs 3 and 5 (assuming no cool down over time) is reasonably conservative, provides margin against the bulk temperature assumed in Reference 22, and does not require any compensatory measure. It is recognized that Attachment B determines an equilibrium flammable concentration that is greater than the existing SB (approximately 10% higher). This is judged to be acceptable based upon the use of the lowest lower flammability limit (LFL) for DMHg in Reference 6. A sensitivity case is provided in Attachment B, utilizing a 2.98% LFL value for DMHg, that reduces the equilibrium flammable concentration below the existing safety basis value by approximately 8%.

The previous discussion/concern is not applicable to SDU 2 or SDU 4. These SDUs are full and will not receive any further radioactive grout. Therefore, it is no longer reasonable to apply the SB flammability models to these locations (i.e., assuming DSA inputs/assumptions). Flammable vapor sample results for SDUs 2 and 4 (Ref. 12 through 19) illustrate that for the material that has already been processed, there are essentially no flammable species in the vapor space. The hydrogen percent of the lower explosive limit is zero percent for all cells and the volatile organic concentrations are all shown to be less than 5.0 ppm. Given that 1 ppm is equal to 0.0001%, it generally takes thousands of ppm for a species to be a flammability concern. As an example, the most conservative LFL for DMHg documented in Reference 6 is 2.5 volume percent. For that LFL value, it would take 25,000 ppm DMHg to reach the LFL. Therefore, based on the sample results and their distance from the LFL, SDUs 2 and 4 are not impacted by the DMHg formation/production or inventory concern previously discussed.

For the SFT, the SB assumes a detonation occurs in this tank. The source term is generated utilizing a trinitrotoluene (TNT) equivalence for a stoichiometric concentration of Isopar L (Ref. 20). Attachment C illustrates that a TNT equivalent detonation for a stoichiometric concentration of DMHg yields approximately 10 percent

greater energy than Isopar L. Since the source term derivation is directly proportional to the energy, a 10 percent increase in energy increases the source term and subsequent consequences by 10 percent. A review of References 3, 5, and 9 determined that increasing consequences by 10 percent does not cause any chemical to exceed its PAC-3 threshold value nor does it cause any additional chemical to exceed 25 percent of its PAC-3 threshold value (i.e., no additional chemicals would be identified as a key hazardous chemical).

To summarize the evaluation provided in this section of the ESS, the compensatory measures provided in PISA PI-2015-0007 (and Section 2.1 of this ESS) may be removed upon DOE approval of this ESS. A new compensatory measure has been identified (provided in Section 2.2) that restricts the cell GROUT height in SDU 3 (Cells A and B) and SDU 5 (Cells A and B). This restriction will not have any adverse facility impacts until the 2017 time frame.

Though not directly related to PISA PI-2015-0007, the results of Reference 2, as it relates to DMHg, indicate an increase in concentration (0.00219 mg/L) above the previous Tank Farm observed maximum concentration (0.00044 mg/L documented in Reference 11). Although the latest results remain significantly below the DSA/WAC value of 1.1 mg/L, it seems prudent to periodically sample for DMHg to ensure it does not reach a point to which the DSA/WAC value is exceeded.

Also not directly related to PISA PI-2015-0007, Reference 6 provides sample results indicating the elemental Hg is present in salt solution. This is not consistent with Reference 23, which is the basis for the chemical forms/concentrations in the current SB. The evaluation below is provided to address this condition and will provide the concentration to reach the PAC-3 threshold for elemental Hg (8.9 mg/m^3).

From Reference 9, the amount of gallons to reach PAC-3 threshold for MMHg (when it was treated as a volatile) is approximately 77,100 gallons (95% met and 3 cm SR). This is based on a PAC-3 threshold value of 2.15 mg/m^3 and a concentration of 1.1 mg/L. From the accidents previously mentioned in the first paragraph of Section 3.1, the highest material at risk quantity is 3530 gallons. This can be seen in Attachment A under the column titled "Volatile ST (gal)" for Consolidated Hazards Analysis (CHA) associated with ELAWD and SDU 3/5. These CHAs comply with the DOE Interim Guidance (95% met and 3 cm SR). The "Facility" CHA (WSRC-TR-2001-00574) values are based on 50% met and 3 cm SR, which would allow an order of magnitude greater source term to exceed PAC. Assuming that this material at risk is equal to the source term, this would equal approximately 4.5% of the PAC-3 threshold value (3530 gallons / 77,100 gallons). At this source term, this would allow a concentration of approximately 24 mg/L to reach the PAC-3 threshold value (1.1 mg/L / 4.5%). Given that the PAC-3 threshold value for elemental Hg is approximately 4.1 times greater than that for MMHg (8.9 mg/m^3 / 2.15 mg/m^3), the allowed concentration of elemental Hg to reach the PAC-3 threshold value is approximately 98 mg/L (24 mg/L X 4.1). The sample results reported in Reference 6 for elemental Hg are significantly below 98 mg/L but indicate a trend upwards. Therefore, as shown in Section 3.3, it is recommended that elemental Hg be added to the WAC as a key chemical.

3.3 Path Forward

1. Implement the compensatory measure provided in Section 2.2 of this ESS and upon DOE approval of this ESS, remove the compensatory measures of PISA PI-2015-0007 (provided in Section 2.1 of this ESS).

2. As an implementation item of this ESS, revise the Saltstone WAC (Ref. 11) for MMHg to a value up to 358 mg/L (DSA value for total Hg) and reference this ESS for the basis (WAC LIMIT). Note that the WAC limit may be further limited due to other considerations (e.g., TCLP). It should be further noted that the evaluation in Section 3.2 identifies other Hg species, potentially present in the liquid waste stream, not currently listed in the DSA or WAC (ethyl, diethyl, dipropyl, dibutyl). The evaluation within this ESS addresses these species such that they do not need to be included in the WAC as an implementation item.

3. As an implementation item of this ESS, revise the Saltstone WAC (Ref. 11) for elemental Hg to a value up to 98 mg/L (WAC LIMIT).

4. Revise, as appropriate, the associated Saltstone analyses and Safety Basis associated with the Higher than Expected Concentration of Methyl Hg in Tank 50 (e.g., Consolidated Hazard Analyses, calculations, inputs/assumptions).

5. As an implementation item of this ESS, revise the Saltstone WAC (Ref. 11) to include periodic sampling of DMHg (WAC TARGET) and total Hg (WAC LIMIT).

3.4 Summary of Recommendations and Conclusions

Based on the results of USQ-SS-2015-00083 and further evaluation of items associated with PISA PI-2015-0007 within this ESS, the PISA compensatory measures are not required for safe operation of the Saltstone Facility. However, the evaluation within this ESS determined that the compensatory measure provided in Section 2.2 is required to be implemented for safe operation of the Saltstone Facility. Furthermore, this ESS will remain in place until a permanent change is made to the SB and associated support documents. The SB change to resolve the Higher than Expected Concentration of Methyl Mercury in Tank 50 PISA (PI-2015-0007) will be submitted to DOE by September 30, 2015.

Attachment A

Evaluation of MMHg as a Non-Volatile Salt

The evaluation provided in this Attachment was performed by reviewing the events in the Saltstone CHAs (Ref. 4, 5, and 7) to find all events involving salt solution. Those events involving heating (i.e., fires and explosions) evaluated the associated source term for MMHg as both a volatile and a precipitate (solid) and determined a concentration equal to the PAC-3 threshold value. For the loss of containment events, only the precipitate (solid) concentration limit was calculated. The calculations for MMHg as a volatile resulted in concentrations to exceed the PAC-3 threshold much less than the 95.2 mg/L (53.5 mg/L applying 2 standard deviations) from sample results. The calculations for MMHg as a precipitate (solid) allow for much higher concentrations before reaching the PAC-3 threshold. Based on Reference 6, the hazards and accident analysis can treat MMHg as a precipitate (solid), which as previously stated, results in chemical consequences far below the PAC-3 threshold value. Therefore, as can be seen by the results, the allowable concentration of MMHg (see column "95% and 3cm Conc. (mg/L) = PAC-3 of 2.15^2"of Attachment) would be limited by the total mercury WAC concentration of 325 mg/L (358 mg/L DSA value).

CHA Listing	Event #	Description	Total SS MAR (gal)[1]	Volatile ST (gal)	95% and 3cm Conc.(mg/L) = PAC-3 of 2.15[2]	50 and 100 Conc (mg/L) = PAC-3 of 2.15[2]	Precipitate ST (gal)	95% and 3cm Conc.(mg/L) = PAC-3 of 2.15[2]	50 and 100 Conc (mg/L) = PAC-3 of 2.15[2]	Comments
Facility	It is not transparent in the fire events whether consequences are calculated for the fire release or if they are solely based on the spill release since there is not a separate ST evaluation/calculation for volatiles. However, they were included here for information purposes and conservatively assumed to be the MAR listed in the CHA event. The Facility CHA is based on 50% and 100 cm for onsite. Did not include NPH Roll-up since it's updated in a later CHA.									
	NODE02-1-0011	Fire in CCBT dike results in spill from transfer line	15000	15000	5.65	52.19	5.29E+00	16024 9	147979.1	Precipitate ST based on possible fire (2 65 gals) and spill (2 64 gals from spill of 20000, only LOC ST given) from S-CLC-Z-00035.
	NODE02-1-0011b	Fire in CCBT dike results in failure of CCBT	500	500	169.54	1565.62				Bounded by NODE02-1-0011
	NODE02-3-0021, -0023, -0041	Failure of salt solution TL	15000	N/A	N/A	N/A	2.64E+00	32110 6	296518.7	The chemical consequences for LOC events in the Facility CHA are based on a MAR of 20000 gal. This bounds all LOC events except the failure of TL and SFT (21504 gal). ST is from S-CLC-Z-00035.
	NODE02-3-0021a, -0023a, -0041a	Failure of IW transfer line	500	N/A	N/A	N/A				
	NODE02-3-0022, -0024, -0042	Failure of CCBT results in spill	500	N/A	N/A	N/A				
	NODE03-1-0011	Fire causes failure of SFT and spill	21504	21504	3.94	36.40	4.00E+00	21193 0	195702 3	The MAR is based on a spill from TL and SFT. The chemical consequences for LOC events in the Facility CHA are based on a MAR of 20000 gal. This bounds all LOC events except the failure of TL and SFT (21504 gal). If burning of SFT occurs, the ST would be .975 gal (S-CLC-Z-00035). Precipitate ST of 4 gal should conservatively bound the larger spill volume with a fire.
	NODE03-2-0012	Explosion in SFT	6504	7513	11.28	104.19	7.64E+00	11095 8	102462 0	STs are from S-CLC-Z-00034.
	NODE03-3-0025	SFT transfer pump results in spill of salt solution	15000	N/A	N/A	N/A	2.64E+00	32110 6	296518.7	The chemical consequences for LOC events in the Facility CHA are based on a MAR of 20000 gal. This bounds all LOC events except the failure of TL and SFT (21054 gal). ST is from S-CLC-Z-00035. For those scenarios with greater than 20000 gallons, a conservative ST of 2.8 gal is used based on volume ratios.
	NODE03-3-0031, -0032, -0033, -7-0034	Overfilling of SFT	15000	N/A	N/A	N/A				
	NODE03-3-0041	SFT empties	6504	N/A	N/A	N/A				
	NODE03-3-0052, -0081, -0082, -0083, -0084, -0085	Failure of TL and SFT causes spill	21504	N/A	N/A	N/A	2.80E+00	30275.7	279574 8	
	NODE04-3-0021	Overflow of mixer	15000	N/A	N/A	N/A	2.64E+00	32110 6	296518.7	
	NODE04-3-0041, -0051, -0052, -0053	Spill of salt solution from TL into 210-Z	15000	N/A	N/A	N/A				
	NODE05-3-0041	Spill of salt solution into 210-Z	15000	N/A	N/A	N/A				
	NODE06-3-0051a	Misalignment of valves during recirc results in spill of SS	6504	N/A	N/A	N/A				
	NODE07-3-0041, -6-002,	Failure of SDU 4 walls results in spill	4000	N/A	N/A	N/A				
	NODE10-1-0011	Fire near leachate return system TL causes release	4000	4000	21.19	195.70				Bounded by SFT fire and spill (NODE03-1-0011)
	NODE10-2-0015	Explosion of leachate return line	4000	4000	21.19	195.70	1.12E+00	75689 2	698936 9	Volatile ST assumed to be equal to MAR. Precipitate ST based on leachate return system explosion (S-CLC-Z-00035).
	NODE10-3-0051, -0061, -0062, -0063	Failure of leachate return line	4000	N/A	N/A	N/A	2.64E+00	32110 6	296518.7	The chemical consequences for LOC events in the Facility CHA are based on a MAR of 20000 gal. This bounds all LOC events except the failure of TL and SFT (21504 gal). For those scenarios a conservative ST of 5 gal is used.
	NODE10A-3-003, -005	Failure of drainwater return line	5700	N/A	N/A	N/A				
	NODE11-6-0014	Aircraft/helicopter crash causes release of salt solution	15000	N/A	N/A	N/A				
	NODE11-6-0015	Aircraft/helicopter crash causes fire and release of salt solution	5700	5700	14.87	137.33	4.70E+00	18036 6	166555 2	Volatile ST assumed to be equal to MAR. Precipitate ST from S-CLC-Z-00035 with some additional volume for 5700 gal vs 4462 gal evaluated
	NODE12-1-002	Fire in drainwater return VB causes failure and release	10000	10000	8.48	78.28	1.62E+00	52328 3	483215.7	Volatile ST assumed to be equal to MAR. Precipitate ST from S-CLC-Z-00035.
	NODE12-3-002	Leachate/drainwater leaks in VB overflowing into SFT dike	10000	N/A	N/A	N/A	2.64E+00	32110 6	296518.7	The chemical consequences for LOC events in the Facility CHA are based on a MAR of 20000 gal. This bounds all LOC events except the failure of TL and SFT (21504 gal). ST is from S-CLC-Z-00035.

CHA Listing	Event #	Description	Total SS MAR (gal)[1]	Volatile ST (gal)	95% and 3cm Conc.(mg/L) = PAC-3 of 2.15[2]	50% and 100 Conc.(mg/L) = PAC-3 of 2.15[2]	Precipitate ST (gal)	95% and 3cm Conc.(mg/L) = PAC-3 of 2.15[2]	50% and 100 Conc.(mg/L) = PAC-3 of 2.15[2]	
ELAWD	In the CHA, there's a general assumption that there isn't enough combustible loading to allow for heating of significant amounts of salt solution in 210-Z process room. Consequences for those events are based on spills. (ELAWD04-3-0012). ELAWD CHA based on 95% and 3 cm for onsite. Events involving full facility inventory were not included since the event MAR is updated in a later CHA. Event MAR and STs taken from A-3 in the CHA.									
	ELAWD04-3-0012	Fire in 210-Z process room	1265				1.67E-01	507616.1	4687481.2	Not enough combustibles for volatile release.
	ELAWD05-3-0051	Mixer discharge outlet plugged causing spill of salt solution	15000	N/A	N/A	N/A	1 98E+00	42814.1	395358.3	
	ELAWD06-2-0014	SHOC explosion	689.5	689 50	122 95	1135.33	6 80E-01	124664.5	1151190.2	Volatile ST based on vapor volume of empty tank.
	ELAWD06-2-0014h	Hopper explosion	516.5	516 50	164.13	1515.60	5 09E-01	166546.0	1537935.9	Volatile ST based on vapor volume of empty tank.
	ELAWD06-3-0024, -0031, -0051, -0085	Spill of salt solution	15000	N/A	N/A	N/A	1 98E+00	42814.1	395358.3	
	ELAWD11-1-0011	Fire in 704-Z spreads to process area, releasing salt solution	1333.4	68.60	1235.74	11411.22	1.74E-01	487194.8	4498904.4	
SDU 3/5	Several events for fires near or in SDUs have assumption that based on construction, there isn't enough combustible material to maintain fire; therefore, there are no releases via fire and no volatile contributions to chemical consequences. SDU 3/5 CHA based on 95% and 3 cm for onsite. Event MAR and STs taken from Table A-8 in the CHA and U-DCF-Z-00013.									
	NODE07C-1-002	HEPA fire	171				2 05E-01	413521.4	3818582.2	
	NODE07C-4-007	Dust/vapor exit cell through penetration	182	N/A	N/A	N/A	3 03E-01	279775.2	2583529.2	
	NODE10C-1-001	Drainwater Return System Spill caused by fire	3530	3530	24 0	221 8	7 08E-01	119734.3	1105662.9	Volatile ST based on 3100 from collection system (1cell) and 430 from return system.
	NODE10C-2-003	Drainwater Collection System Explosion	351.5				3 35E+00	25305.0	233674.4	
	NODE10C-3-001, -002	Drainwater Return System Leak	750	N/A	N/A	N/A	7 85E-01	107989.7	997209.4	The MAR is based on 4 drainwater collection system cells and the return line. Resuspension is based on 12830 gal.
	NODE11-6-0012	Wildland Fire	547	547	155 0	1431.1	7 21E-02	1175754.4	10857272.7	Volatile ST based on volumes from HEPAs.
	NODE11-6-0012-3/5	Wildland Fire (only 3/5)	171	171	495.7	4577 8	2 25E-02	3767639.7	34791527.1	
	NODE11-6-0013	Vehicle impact into facility structure (Salt Solution) and fire	15000	15002	5.7	52 2	4 54E+00	18672.2	172425.0	
	NODE11-6-0013	Vehicle impact into facility structure (process room) and fire	806	N/A	N/A	N/A	4.63E+00	18309.3	169073.3	
	NODE11-6-0016	Aircraft/Helicopter crash into exposed TL	17330	3530	24 0	221 8	7 85E-01	107989.7	997209.4	
	NODE11-6-0017	Vehicle impact into exposed TL	3530	3530	24 0	221 8	7 08E-01	119734.3	1105662.9	
	NODE11-6-0018	Crane failure impacts exposed TL	17330	N/A	N/A	N/A	6 80E-01	124664.5	1151190.2	
	NODE11-6-0018c	Crane failure impacts cell roof	3282	N/A	N/A	N/A	8 32E-01	101889.3	940876.6	
	NODE11-6-0019	Vehicle driven on roof	171	N/A	N/A	N/A	2.73E-01	310519.8	2867433.6	
	NODE11-7-0021	Tornado/high winds		15002	N/A	52 2	5 02E+01	N/A	15593.8	MAR is full facility inventory for NPH roll-up.
	NODE11-7-0021-3/5	Tornado/high winds - sdu only	87257	N/A	N/A	N/A	8 29E-01	102258.0	944281.5	
	NODE11-7-0026	Seismic event		15002	N/A	52 2	1 04E+01	N/A	75270.1	MAR is full facility inventory for NPH roll-up.
	NODE11-7-0026-3/5	Seismic event - sdu only	87257	N/A	N/A	N/A	1.71E+00	49574.2	457783.3	

Footnotes:

1. The material at risk (MAR) is taken from the Hazard Evaluation table event in the specified CHA. Due to the nature of some of the events, multiple volumes are listed under the MAR in the HE tables in order to take into account event durations. For example for chemical consequences, smaller event durations were considered such that for a Loss of Containment event the pump rate would be multiplied by 15 minutes resulting in a much smaller volume than the entire system volume.
2. The PAC value is based on Rev. 26 of the PACs for Chemicals of Concern (used in S-CLC-Z-00088, Rev. 2). The methyl mercury concentrations to reach PAC-3 were calculated by multiplying the PAC-3 threshold by the event duration (15 min, or 900 sec) then dividing by the χ/Q, the conversion from gallons to liters (3.7854 L/gal), and the event source term. This calculation was based on those performed in S-CLC-Z-00088. The χ/Q values are 6.03E-03 s/m^3 for 95th percentile and 3 cm surface roughness and 6.53E-04 s/m^3 for 50th percentile and 100 cm (S-CLC-Z-00065 Rev. 1).

Attachment B

Impacts of DMHg on SDU 3 and 5 Flammability

Introduction

Flammable methylated mercury compounds have historically not been included in SDU flammability analyses (see, e.g., Reference 1). Recent work (Reference 2) has identified four dialkyl mercury species as potential constituents in the SDU vapor space. This attachment assesses the effect of those species on the flammability of SDU 3/5. The analysis detailed here provides a bounding treatment for the purpose of establishing a short-term compensatory measure. It is expected that a future revision to Reference 1 will be issued that addresses flammable mercury compounds at a level of rigor commensurate with the previous analysis so that the compensatory measure determined here may be relaxed or removed.

Analysis/Discussion

The analysis documented in Reference 1 includes the flammable species shown in Table B-1. Table B-1 presents the Reference 1 inputs related to these flammables and the inputs used in the present attachment, as discussed/justified later in the attachment.

Table B-1. Inputs for Flammable Species

Species	Reference 1		Current Attachment	
	Salt Solution	Premix	Salt Solution	Premix
Ammonia	200 mg/l	-	200 mg/l	-
Benzene	4.15 kg	0.13 mg/g saltstone	4.15 kg	0.13 µg/g saltstone
Butanol	1.03 mg/l	-	1.03 mg/l	-
Hydrogen	1.41E-08 ft^3/hr/gal @ 95° C	-	1.41E-08 ft^3/hr/gal @ 95° C	-
Dimethylmercury	-	-	1.1 mg/l [Note 1] 9.02E-08 ft^3/hr/gal @ 95° C [Note 2]	-
Isopar L	11 ppm	-	11 ppm	-
Isopropanol	0.25 mg/l	-	0.25 mg/l	-
Methanol	0.25 mg/l	-	0.25 mg/l	-
Norpar 13	0.1 mg/l	-	1 mg/l	-
Toluene	-	1.667µg/g saltstone	-	1.667µg/g saltstone
Xylene	40 g/hr of pour	10% of Toluene	40 g/hr of pour	10% of Toluene

Note 1: Modeled as isopropanol.
Note 2: Modeled as hydrogen.

The value of 9.02E-08 ft^3/hr/gal is calculated as follows:

V_{molar}

$$V_{molar}(95\deg C)=\left(\frac{273.15+95}{273.15}\right)V_{molar}(0\deg C)=\left(\frac{273.15+95}{273.15}\right)V_{molar}(22.414)=30.21 l/mole$$

DMHg Rate

$$R_{DM}=\left(358\frac{mg}{l}\right)(4.0E-09/s)=1.43E-06 mg/l/s$$

$$R_{DM}=\left(1.43E-06\frac{mg}{l*s}\right)\left(\frac{1}{1000}\frac{g}{mg}\right)\left(\frac{1}{230.7}\frac{mole}{g}\right)\left(\frac{1}{0.26417}\frac{l}{gal}\right)\left(30.21\frac{l}{mole}\right)\left(0.03531\frac{ft^3}{l}\right)\left(3600\frac{s}{hr}\right)$$

$$R_{DM}=9.02E-08\frac{ft^3}{gal*hr}$$

Ammonia is assumed to be present in the vapor space at a constant bounding concentration. Hydrogen is assumed to be generated continuously via radiolysis at a constant specific rate. The other gases have fixed inventories in the grout and are therefore depleted as the scenario progresses. Isopar L, benzene, xylene, and toluene are modeled as diffusive releases from the grout. The alcohols and Norpar 13 are released immediately upon pouring.

The SDU vapor space is assumed to be well-mixed based on convective flow when the grout surface is hotter than the roof and based on CFD studies when the roof is hotter than the surface. As discussed in Reference 1, a layer of Isopar L on the surface when the roof is hotter than the surface will dissipate in about 10 minutes. Based on the diffusion coefficient of elemental mercury, the diffusion coefficient of DMHg is expected to be lower than that of Isopar L by a factor of two or three. Therefore, a DMHg layer would be expected to take longer to dissipate. However, a longer dissipation time, say on the order of an hour or two which might be implied by the difference in diffusion coefficients, would not alter the conclusion that the vapor space was well mixed.

In the bounding scenario, the SDU is filled from empty to a final fill height of 21.76 ft using 27 straight 10-hr pour days. The resulting peak concentration of flammables is 99.7 % CLFL. This peak doesn't occur until day 350 and is composed primarily of hydrogen (at 57 %CLFL) and Isopar L (at 27 %CLFL). The delay in reaching the peak is caused primarily by the slow diffusion of Isopar L from the grout. Because of this delay, the calculated concentration is insensitive to the pour schedule. The final equilibrium concentration of flammables in the vapor space, composed of hydrogen and ammonia, is 75.3 % CLFL.

Without modifications to the methodology, mercury species can be included in the analysis in two ways. If a fixed concentration in salt solution is known, the species can be released immediately upon pouring in the same way that the alcohols and Norpar 13 are released. Alternatively, if a production (and release) rate of the species is known, it can be modeled in the way that hydrogen is modeled, i.e., using a constant specific release rate. If modeled as a rate, the species contributes to the final equilibrium concentration as well as to the peak concentration.

Dimethylmercury (DMHg), which is the bounding species (from a flammability standpoint) identified in Reference 2, has been included in previous Saltstone Production Facility (SPF) chemical consequence analyses at a concentration of 1.1 mg/liter of salt solution (Reference 3). Samples of SDU 2 and SDU 4 vapor spaces indicate concentrations of organics on the order of a few ppm (see, e.g., Reference 4). In the bounding Reference 1 scenario described previously, the vapor space volume is 147 m^3 and the grout volume is 11,000 m^3. If it is assumed that the entire 11,000 m^3 of grout contains 1.1 mg/l of DMHg in salt solution and that this DMHg is released completely into the 147 m^3 vapor space, the resulting concentration would be 0.8 %. This value is orders of magnitude above any of the measured concentrations. Even allowing for variations in the timing/location of the measurements and in actual versus allowed concentrations of mercury compounds in salt solution, the 1.1 mg/l concentration is extremely conservative; therefore, it is assumed here to represent all flammable mercury compounds, not just DMHg.

According to Reference 5, DMHg may be formed at a rate that depends on the total concentration of mercury present. Recent measurements discussed in the main body of this ESS indicate that the salt solution making up incoming grout may have a total mercury concentration as high as 358 mg/l. For the present analysis, a production rate of 4.0E-09/s times the total mercury inventory is used. This rate constant is the value given in Reference 5 for 81°C, which represents a reasonably conservative value for the temperature of the grout monolith. The rate determined in this way is extremely conservative based on comparison with actual measurements of flammables in the vapor space (see, e.g., Reference 4) as follows: Assuming only a month of production at the minimum rate given in Reference 5 (which corresponds to a temperature of 39° C) and a total mercury concentration of 1.1 mg/l in salt solution, the calculated DMHg concentration in the vapor space is 0.0013% at the limiting SDU 3/5 configuration. This value is orders of magnitude above the measured concentrations. A total mercury concentration of 358 mg/l combined with the maximum rate discussed previously and a longer generation time would give a calculated concentration that is orders of magnitude higher than 0.0013%. Based on these considerations, the rate of DMHg production determined above (4.0E-09/s times a total mercury concentration of 358 mg/l) is assumed to include the production of all flammable species of mercury, not just DMHg.

The bounding scenario analyzed in this attachment includes DMHg and total mercury at concentrations of 1.1 mg/l and 358 mg/l, respectively, in the salt solution making up the incoming grout. The rate of DMHg production is based on 4.0E-09/s times the total mercury inventory. As justified in the previous paragraphs, DMHg is assumed to represent all flammable mercury species. The allowed grout fill height in SDU 3/5 is determined such that the concentration of flammables in the vapor space remains comfortably below 100% CLFL.

DMHg present in the incoming grout is modeled as isopropanol. This is conservative because the LFL of isopropanol (2.2 %) is lower than that of DMHg determined in Reference 2 (2.5% based on assuming DMHg can be represented as two methanes). (The heats of combustion of the two species are similar; therefore, the isopropanol LFL remains below that of DMHg after temperature correcting.) The concentration of isopropanol used in Reference 1 (0.25 mg/l) is increased to 0.25 + 1.1 = 1.35 mg/l).

DMHg produced from the total mercury present in the incoming grout is modeled as hydrogen. Because the LFL of hydrogen at 25° C (4 %) is higher than that of DMHg (2.5%), to bound the effect of DMHg, the LFL of hydrogen in the calculation is set to 2.5%. The rate of DMHg production (concentration * rate constant discussed above) is added to the hydrogen generation rate.

If the final fill height is set to 19.25 ft, the concentration of flammables in the vapor space as a function of time is given in Figure B-1. The concentration of flammables in the vapor space is still increasing at 1000 days. The extension of the workbook to address times longer than 1000 days could not be done given schedule constraints. The concentration of flammables at 1000 days is 83.4 %CLFL. The shape of the curve, however, is such that the ultimate peak will remain below 100 %CLFL. The equilibrium concentration is calculated independently from the concentration-time curve. The equilibrium concentration is 82.5 %CLFL. This scenario includes an inadvertent transfer of 15,000 gallons of salt solution.

Additional Sensitivity Case

An additional case was analyzed to examine the effect of increasing the assumed LFL of DMHg to 2.98% (based on a flashpoint of 5°C as shown in Reference 1). The result is a concentration at 1000 days of 70.9 %CLFL and an equilibrium concentration of 69.8 %CLFL.

Conclusion

The bounding case presented in this attachment indicates that establishing a fill height limit of 19.25 ft for SDU 3/5 is adequate to protect 100 %CLFL with the addition of flammable mercury species to the flammable species already considered in the SDU 3/5 analysis.

References

1. Saltstone Facility SDU 2 and SDU 3/5 Flammability Analysis (U). S-CLC-Z-00080, Rev. 1, August 2013.
2. Volatilization and Flammability Characteristics of Elemental and Organic Mercury. X-ESR-G-00048, Rev. 1, May 2015.
3. Saltstone Facility Input Data Base, Item SF-I-PC-0049, Rev. 0.
4. "IH Baseline Monitoring for Combustible Atmosphere for SDU 4", SRR-FSH-00003", May 2014.
5. "Kinetic Treatment of Dimethyl Mercury Degradation and Formation Studies", SRNL-WHM-2004-00006, Rev. 0, September 2004.

6.

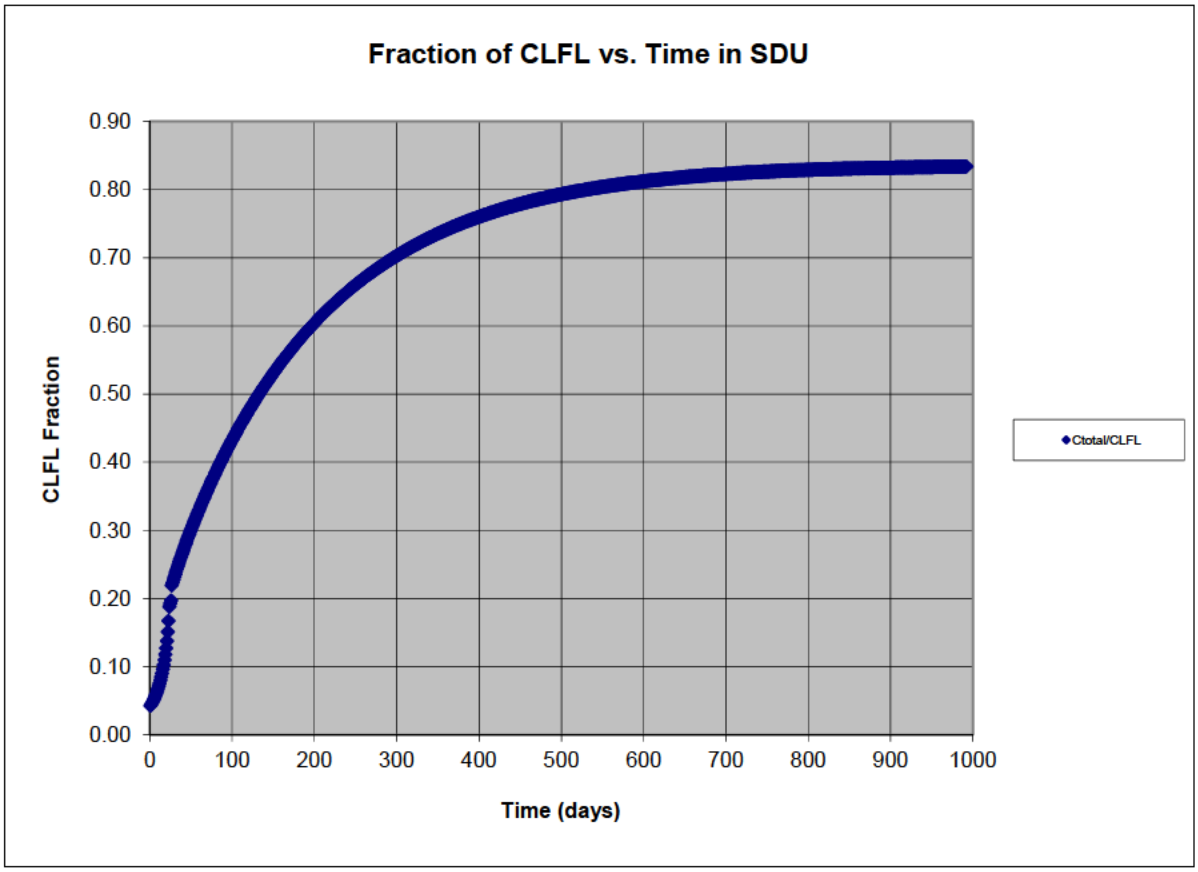


Figure B-1. Fraction of CLFL vs Time including DMHg at a Final Fill Height of 19.25 ft in SDU 3/5.

Attachment C

TNT Equivalent of DMHg

TNT Equivalent of Dimethyl Mercury

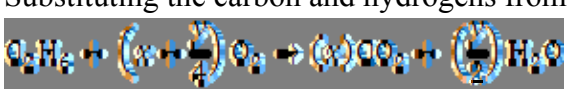
Based on the methodology presented in S-CLC-Z-00070 (Ref. 1), a similar calculation is performed here to determine the TNT equivalent mass of DMHg in a volume of 100 L and compare the mass to the TNT equivalent mass of the current bounding flammable Isopar L. In order to calculate the TNT equivalent mass, the following inputs and methodology are used:

Input 1: Oxygen accounts for only 21% of the concentration in air (Ref. 1).
Input 2: The energy produced from 1 gram of TNT is 1.1 kcal (Ref. 1).
Input 3: The volume of one mole of ideal gas is 22.4 mol/L and corrected to 25°C is 24.4513 mol/L.
Input 4: Dimethyl Mercury Properties

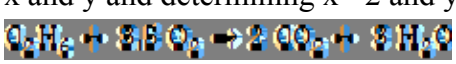
Chemical	Chemical Formula	Stoichiometric Percent in Air[1]	MW [g/mol][2]	Heat of Combustion [kJ/mol][2]
Dimethyl Mercury	$(CH_3)_2Hg$	6.00%	230.66	1806.7

1. The stoichiometric percent in air is calculated using the simple combustion model given in Reference 1 and is shown below:

Substituting the carbon and hydrogens from the dimethyl mercury results in the following:



Based on the 2 carbon atoms and 6 hydrogen atoms, the chemical equation can be balanced solving for x and y and determining x= 2 and y=6 resulting in the following balanced equation:



Using the ratio of moles of oxygen to moles of fuel, the stoichiometric concentration can be calculated.

Total volume = 100 L
O_2 volume = 0.21 * Total volume = 0.21 * 100L = 21 L
Moles of O_2 = 3.5
Moles of Dimethyl = 1

$$\text{Molar ratio} = \frac{\text{Moles of Dimethyl}}{\text{Moles of } O_2} = \frac{1}{9.5}$$

$$\text{Volume of Dimethyl} = O_2 \text{ volume} * \text{Molar ratio} = 21\text{ L} * \frac{1}{9.5} = 6\text{ L}$$

Stoichiometric concentration = $\frac{\text{Volume of dimethyl}}{\text{Total Volume}} = \frac{6\text{ L}}{100\text{ L}} = 0.06$ or 6%

2. The molecular weight and heat of combustion for dimethyl mercury were taken from Reference 2. In order to convert to kcal/mol, the unit conversion of 0.23901 is used and results in a heat of combustion of 431.81 kcal/mol.

To determine the TNT equivalent mass, the following equation is used.

$$M = \frac{V_{tank} * V_{fraction} * E_c}{V_{ideal} * E_{TNT}}$$

Where,

M	=	TNT mass equivalent
V_{tank}	=	vapor volume of tank, 100 L
$V_{fraction}$	=	stoichiometric volume fraction, 0.06
E_c	=	heat of combustion, 431.81 kcal/mol
V_{ideal}	=	volume of one mole gas, 24.4513 mol/L
E_{TNT}	=	energy of 1 g of TNT, 1.1 kcal/g

This results in a TNT mass equivalent of 96.33 g, which is greater than the 87.33 g given in Reference 1.

References:

1. TNT Equivalence for the Complete Combustion of Select Chemicals in Air (U). S-CLC-Z-00070, Rev. 0.
2. *Mercury, dimethyl-*, National Institute of Standards and Technology Chemistry WebBook, http://webbook.nist.gov/cgi/cbook.cgi?ID=C593748&Mask=69F.