A CST Waste Tank Accident Analysis for a Post-Seismic Explosion Event

M. R. Yeung
D. C. Thoman
K. H. Barbour

URS Safety Management Solutions LLC
2131 S. Centennial Ave.
Aiken, SC 29803
ray.yeung@wsms.com

Abstract

An analysis has been conducted to define a bounding tank to represent the 51 waste storage tanks at the Concentrate Storage and Transfer (CST) Facility of the Savannah River Site (SRS) for the seismic follow-on explosion event. This bounding tank is used to perform the accident analysis to investigate the consequence of the explosion for two scenarios. Analytical models have been developed to determine the hydrogen concentration in the tank vapor space as a result of radiolysis generation and sudden release of the hydrogen trapped in the sludge and saltcake. This analysis also investigates the consequences caused by hydrogen deflagration and detonation. The results of the analysis indicate that the offsite dose of such an event is limited to approximately 2.1 rem.

Introduction

The CST Facility located in the F and H Areas of SRS houses 51 tanks used for nuclear waste storage. At the time this paper is prepared, 12 of these tanks have been grouted, in the process of closure, or currently under the Q-time program. (The Q-time program identifies tanks with rapid hydrogen generation rates and provides extra control of flammable gas conditions through regular agitation of the sludge layer to release trapped gas). Therefore, only 39 of these tanks are modeled in this analysis. By design, these tanks can be categorized into 4 major types; namely, Type I, Type II, Type III/IIIA, and Type IV. Some of these tanks hold only supernate (liquid waste form), while some others have settled sludge and saltcake. An overall summary of the present status of the CST tanks is given in Table 1, which shows the levels and densities of the sludge, saltcake, and supernate of each of these tanks. Table 1 also shows the Inhalation Dose Potentials (IDPs) of each individual tank.
During a seismic event, it is postulated that the tank ventilation system is disabled, resulting in hydrogen buildup in the tank vapor space due to continuous radiolysis of the
waste. The hydrogen accumulation is further exacerbated by the sudden release of the hydrogen originally trapped in the sludge and saltcake prior to the earthquake. With the presence of an ignition source, an explosion can occur if the hydrogen concentration exceeds its flammability limit. Although it is possible to perform accident analyses for each of the tanks, it is judged that the explosion consequence of a “bounding tank” can be used to represent all classes of tanks of the entire CST facility. The purpose of this paper is to present the methodology used to define the bounding tank and the mathematical model used to analyze the consequence of an explosion following a seismic event. The result of this study is used as the Safety Basis of the CST Facility.

Mathematical Model Used for Analysis

Defining the Bounding Tank for Analysis

Since the explosion energy is proportional to the combustible gas volume, the larger tank types potentially yield the worst consequences. Among all tank types, the Type IV tank has the largest volume but analysis has shown that hydrogen generation with bounding waste at its fill limit does not produce enough hydrogen in seven days to reach the Lower Explosivity Limit (LEL) of 12 vol%. With the Type III/IIIA tanks as the next largest, the analysis of this paper shows that the hydrogen concentration can reach the stoichiometric concentration of 29.5 vol% for the bounding waste. Therefore, the Type III/IIIA dimensions are used for the bounding tank analysis. The present analysis pursues the investigation of the explosion consequence in two scenarios:

- Scenario A - characterized by a configuration of 90 inches of settled sludge with no saltcake
- Scenario B - characterized by a configuration of 40 inches of settled saltcake and 50 inches of settled sludge.

For each scenario, supernate is assumed to cover the settled sludge and saltcake (if present), and its level is varied parametrically up to the fill limit. According to Table 1, 15 tanks have only sludge (with supernate) and no saltcake. Among this group, Tank 26F has the maximum 82.63 inches of sludge while Tank 13H has the second highest thickness of 81.75 inches. Since there are no plans for either one of these two tanks to receive any more new sludge, the choice of 90 inches for sludge thickness for Scenario A is reasonable. The remaining 24 tanks have both sludge and saltcake with various configurations – i.e., sludge on top or bottom (and with or without supernate). As Reference 3 points out that trapped hydrogen release from the saltcake is only observed up to the level of 40 inches, this means that incremental increases of saltcake thickness beyond 40 inches do not lead to additional hydrogen release. Tank 32H and Tank 47F have respectively 29.55 inches and 70.65 inches of sludge, but they are both trapped under layers of saltcake greater than 40 inches. Therefore, Tank 33F, with 83.7 inches of saltcake and 20.5 inches of sludge on top of it, is the most limiting tank for Scenario B. With the bounding scenarios defined, the key inputs used for the analysis are summarized in Tables 2a and 2b.
### Table 2a – Key Inputs used in the Analysis [Ref. 3]

<table>
<thead>
<tr>
<th>Input Description</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bounding tank</td>
<td>Type III/IIIA</td>
<td></td>
</tr>
<tr>
<td>Scenario A: Sludge layer thickness</td>
<td>90</td>
<td>inches</td>
</tr>
<tr>
<td>Saltcake thickness</td>
<td>0</td>
<td>inches</td>
</tr>
<tr>
<td>Scenario B: Sludge layer thickness</td>
<td>50</td>
<td>inches</td>
</tr>
<tr>
<td>Saltcake thickness</td>
<td>40</td>
<td>inches</td>
</tr>
<tr>
<td>Tank volume</td>
<td>1,373,238</td>
<td>gal</td>
</tr>
<tr>
<td>Tank height</td>
<td>396</td>
<td>inches</td>
</tr>
<tr>
<td>Tank radius/diameter</td>
<td>42.5/85</td>
<td>inches</td>
</tr>
<tr>
<td>Tank fill limit</td>
<td>372</td>
<td>inches</td>
</tr>
<tr>
<td>Supernate density</td>
<td>1.6</td>
<td>kg/L</td>
</tr>
<tr>
<td>Settled sludge density</td>
<td>2.5</td>
<td>kg/L</td>
</tr>
<tr>
<td>Saltcake density</td>
<td>1.3</td>
<td>kg/L</td>
</tr>
<tr>
<td>Initial tank temperature</td>
<td>25</td>
<td>°C</td>
</tr>
</tbody>
</table>

### Table 2b – Fill Limit for Type III/III Tanks [Ref. 3]

<table>
<thead>
<tr>
<th>Input Description</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tank fill factor (&lt; 300 inches)</td>
<td>3510</td>
<td>gal/inch</td>
</tr>
<tr>
<td>Waste Volume for Tank Levels ≥ 300 inches (V\textsubscript{waste})</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• 325 inches</td>
<td>1,140,298</td>
<td>gal</td>
</tr>
<tr>
<td>• 334 inches</td>
<td>1,171,471</td>
<td></td>
</tr>
<tr>
<td>• 342 inches</td>
<td>1,199,041</td>
<td></td>
</tr>
<tr>
<td>• 354 inches</td>
<td>1,240,120</td>
<td></td>
</tr>
<tr>
<td>• 366 inches</td>
<td>1,280,824</td>
<td></td>
</tr>
<tr>
<td>• 372 inches</td>
<td>1,301,021</td>
<td></td>
</tr>
</tbody>
</table>

### Flammability Analysis for Hydrogen in Tank Vapor Space

The flammability analysis calculates the build up of hydrogen in the tank vapor space just prior to the explosion to establish the \( \text{H}_2 \) vapor space concentration to determine whether a deflagration or detonation occurs, and to use it for calculation of the combustion energy.

The three potential sources of hydrogen are: (1) the initial \( \text{H}_2 \) in the vapor space, (2) trapped-gas \( \text{H}_2 \) releases from the settled sludge layer and saltcake layer (if present) as a result of the agitation caused by the seismic activities, and (3) radiolytic \( \text{H}_2 \) generation from sludge and supernate. Additionally, organic vapors in the tank are modeled in terms of an effective hydrogen concentration. In this analysis, the tank is assumed to be isolated, except for diurnal breathing. Mathematically, the cumulative hydrogen concentration in the tank vapor space on the seventh day after the seismic event can be expressed as:

\[
Y_{\text{H}_2} = Y_{\text{H}_2,7d} + Y_{\text{H}_2,\text{org}} + (Y_{\text{H}_2,o} + F_{\text{exp}}Y_{\text{H}_2,\text{tg}})\cdot(f_{\text{diurnal}})^6
\]  \hspace{1cm} (1)

where

\( Y_{\text{H}_2,7d} \quad \text{Radiolytic (7-day) H}_2 \text{ contribution to vapor space concentration} \)
\[ Y_{H2,\text{org}} = \text{Effective } H_2 \text{ concentration in vapor space for organics} \]
\[ Y_{H2,o} = \text{Initial } H_2 \text{ concentration in vapor space} \]
\[ Y_{H2,\text{tg}} = \text{Trapped-gas release } H_2 \text{ contribution to vapor space concentration} \]
\[ F_{\text{exp}} = \text{Volume expansion factor for released trapped gas} \]
\[ f_{\text{diurnal}} = \text{Daily breathing reduction factor} \]

Per Facility control, the concentration of the hydrogen in any tank vapor space has to be kept within 4 vol% at the end of the 7-th day. This implies that the sum of \( Y_{H2,o} \) and \( Y_{H2,7d} \) is controlled to a maximum value of 0.04. It is conservative to set \( Y_{H2,7d} \) to 0.04 and \( Y_{H2,o} \) to zero as \( Y_{H2,7d} \) is not reduced by the diurnal breathing effect. With these specifications, one can easily see that \( Y_{H2,7d} \) is equal the Lower Flammability Limit (LFL) concentration of 4 vol% at 25°C [Ref. 4] and that trapped gas releases and the presence of organics are thus responsible for tank vapor space concentrations above LFL in the analysis. For this analysis, the contribution to the hydrogen concentration by the organics is equivalent to 0.96 vol% \( H_2 \) [Ref. 3] and the diurnal breathing factor is 0.9951 [Ref. 5].

The trapped gas release contribution to the hydrogen concentration \( Y_{H2,\text{tg}} \) can be calculated by the following equation:

\[ Y_{H2,\text{tg}} = \frac{\left( v_{H2,\text{sl}} h_{\text{sl}} + v_{H2,\text{sc}} h_{\text{sc}} \right)}{V_g}, \quad (2) \]

where
\[ v_{H2,\text{sl}} = \text{volume of } H_2 \text{ released from sludge per inch depth of the sludge} \]
\[ v_{H2,\text{sc}} = \text{volume of } H_2 \text{ released from saltcake per inch depth of the saltcake} \]
\[ h_{\text{sl}} = \text{height of the sludge} \]
\[ h_{\text{sc}} = \text{height of the saltcake} \]
\[ V_g = \text{tank vapor space volume} = V_{\text{tank}} - V_{\text{waste}} \]
\[ V_{\text{tank}} = \text{tank volume} \]
\[ V_{\text{waste}} = \text{liquid waste volume} \]

Note that the waste volume can be directly calculated by the liquid level by the fill factor if it is less than 300 inches. For liquid level higher than 300 inches, the waste volume must be looked up from the input table. The general expression for the volume of the trapped hydrogen released from a unit depth of sludge or saltcake is:

\[ v_{H2} = f_{\text{void}} f_{H2} f_{\text{rel}} V_{\text{ff}}, \quad (3) \]

where
\[ f_{\text{void}} = \text{void fraction} = \begin{cases} 0.1 & \text{for sludge} \\ 0.11 & \text{for saltcake} \end{cases} \quad [\text{Ref. 3}] \quad (4) \]
\[ f_{H2} = \text{hydrogen fraction in void space} = 0.5 \quad [\text{Ref. 3}] \quad (5) \]
\[ V_{\text{ff}} = \text{tank fill factor} = 3,510 \text{ gal/in} \]
The release fraction, $f_{rel}$, is given by:

$$f_{rel} = \begin{cases} 
0.5 \times \frac{h_{waste}}{400} & \text{for sludge} \\
0.5 & \text{for saltcake}
\end{cases} \quad [\text{Ref. 3}] \quad (6)$$

and $h_{waste} =$ total height of sludge and saltstone, in inches.

Note that the total height $h_{waste}$ given in Equation (6) was originally developed for sludge only. This analysis conservatively applies it for both sludge and saltcake, regardless of the orientation or configuration of the physical arrangement of the sludge and saltcake. By the same token, the release fraction of the saltcake is also set to 0.5 for the entire 40 inches, regardless of the configuration of any physical arrangement of the sludge and saltcake. With Equation (3) substituting into Equation (2), the hydrogen concentration contributed by the trapped gas can be determined.

Since the trapped gas is released below the liquid surface, it experiences a gradual reduction of hydrostatic pressure as it ascends to the surface. As a result, the trapped gas is expected to expand in a manner proportional to the ratio of the hydrostatic pressure at the release location and the atmospheric pressure. For the supernate-on-top sludge configuration (i.e., Scenario A), the expansion factor is:

$$F_{exp \_ A} = 1 + \left( \frac{\rho_{\text{sup}} h_{\text{liq}} + 0.5 \rho_{\text{sl}} h_{\text{sl}}}{P_0} \right) g \left( \frac{1000 \frac{L}{m^3}}{0.0254 \frac{m}{in}} \right) \quad (7)$$

where

- $\rho_{\text{sup}} =$ supernate density, in kg/L
- $\rho_{\text{sl}} =$ sludge density, in kg/L
- $h_{\text{liq}} =$ supernate height, in inches
- $h_{\text{sl}} =$ sludge height, in inches
- $g =$ gravity constant = 9.81 m/s$^2$
- $P_0 =$ atmospheric pressure = 101,325 Pa.

For a tank with the supernate on top, settled sludge in the middle, and the saltcake on the bottom (i.e., Scenario B), the following expansion factor is used:

$$F_{exp \_ B} = 1 + \left( \frac{\rho_{\text{sup}} h_{\text{liq}} + \rho_{\text{sl}} h_{\text{sl}} + 0.5 \rho_{\text{sc}} h_{\text{sc}}}{P_0} \right) g \left( \frac{1000 \frac{L}{m^3}}{0.0254 \frac{m}{in}} \right) \quad (8)$$

where

- $\rho_{\text{sc}} =$ saltcake density, in kg/L
- $h_{\text{sc}} =$ saltcake height, in inches.

Note that this expansion factor is applied to both sludge and saltcake, regardless of the physical configuration. With the expansion factor determined, the total hydrogen concentration can be evaluated by simply substituting Equations (7) and (2) into Equation (1).
Calculation of Explosion Energy

With the concentration of hydrogen in the tank vapor space known, the energy released from the total combustion of the hydrogen is:

\[ E_{H_2} = N_{H_2} \cdot H_{c,H_2} \left( 4.1868 \frac{kJ}{kcal} \right), \]  

(9)

where

\[ H_{c,H_2} = \text{heat of combustion of hydrogen} = 57.8 \text{ kcal/mol} \quad [\text{Ref. 4}] \]

The number of moles of hydrogen, \( N_{H_2} \), is given by:

\[ N_{H_2} = \frac{Y_{H_2} \cdot V_g}{V_m} \left( 3.785 \frac{L}{gal} \right), \]  

(10)

where \( V_m \) is the standard molar volume (22.4 L/mol) corrected to the operating temperature. This analysis disables and suppresses the combustion energy calculation if the hydrogen concentration is below its LFL of 4 vol% [Ref. 4]. On the other hand, if the hydrogen concentration is above its stoichiometric concentration of 29.5% [Ref. 4], this analysis caps the combustion energy at the stoichiometric concentration.

Calculation of the Source Term

When the hydrogen concentration is between 4 and 12 vol%, this analysis uses the deflagration model to evaluate the source term, which is given in the following equation:

\[ ST_{def} = \frac{f_A \cdot E_{H_2} \cdot (ARF \times RF)}{h_{fg} \left( 3.785 \frac{g}{gal} \right)}, \]  

(11)

where

\[ ST_{def} = \text{deflagration source term in gal} \]
\[ f_A = \text{fraction of combustion energy being deposited on liquid} \]
\[ h_{fg} = \text{heat of vaporization for water} = 2.257 \text{ kJ/g} \]
\[ ARF = \text{airborne release fraction} = 0.1 \]
\[ RF = \text{respirable fraction} = 1 \]
\[ 3,785 = \text{density of water [g/gal]} \]

The rationale of using 0.1 for the Airborne Release Fraction (ARF) is based on the DOE-3010-94 Guidebook [Ref. 6], which suggests the value of 0.1 may be used for venting of liquid with 50 to 100°C superheating. In a deflagration, heat transfer from the combusted gases to the liquid is basically the radiant mode. Without internal heat source within the liquid, it is difficult to have superheating. Thus one can expect that it creates less
entrainment (by bubbles) than that from the flashing process and using an ARF of 0.1 is reasonable.

The energy fraction $f_A$ is calculated by the geometric ratio of the liquid surface area and the total surface area, i.e.,

$$f_A = \frac{A_{liq}}{A_{liq} + A_{walls} + A_{roof}}$$

(12)

where

- $A_{liq} =$ surface area of the liquid “seen” by the combusted gases
- $A_{walls} =$ side wall surface area exposed to the combusted gases
- $A_{roof} =$ roof (tank top) surface area exposed to the combusted gases.

The use of the surface area ratio implies that these surfaces are treated as black bodies such that all energy incident on them is absorbed and none is reflected back toward other surfaces. In reality, it is true that no surfaces are 100% black and all surfaces are, to various degrees, gray and they exchange heat with each other by reflection or re-radiation. Since none of the side walls or the roof has been specially polished to create a preferential reflection pattern for radiation heat toward the liquid surface, it is reasonable to expect the reflection of radiative heat is basically diffuse (non-directional). On the other hand, the temperatures of the walls and the liquid are generally low compared to the combusted gases, such that heat exchange by re-radiation would be small compared to that from the combusted gases. As a result, it is clear that treating all surfaces as black bodies actually is conservative because it minimizes the energy in the vapor space and maximizes the heat deposited on the liquid. The conservatism of the analysis is further enhanced as the energy is assumed to be absorbed in a thin layer at the surface for its complete vaporization.

When the hydrogen concentration is equal or greater than the hydrogen LEL of 12 vol% [Ref. 7], this analysis assumes the occurrence of detonation and uses the TNT model to evaluate the source term [Ref. 6], which is given in gal as follows:

$$ST_{det} = \frac{E_{H_2}}{E_{TNT} \left[ 4.1868 \frac{kJ}{kcal} \right] \left[ \rho_{slurry} \left( 3.785 \frac{L}{gal} \right) \left( 1000 \frac{g}{kg} \right) \right]}$$

(13)

where

- $E_{TNT} =$ specific TNT energy = 1.1 kcal/g [Ref. 6]
- $\rho_{slurry} =$ waste slurry density in kg/L.

The term “slurry” here refers broadly to any mixture of liquid supernate and sludge solids to emphasize the two components. The detonation source term $ST_{tet}$ given Equation (12) is gallon waste slurry. With the source term determined, the offsite dose, in rem, is simply the product of the source term and the unit dose factor; i.e.,
\[ Dose_{MOI} = ST \times TEDE_{slurry} \]  

where
\[
ST = \text{either } ST_{def} \text{ or } ST_{tet}, \text{ in gal}
\]
\[
TEDE_{slurry} = \text{unit dose factor for waste slurry, in rem/gal.}
\]

In this analysis, the TEDE is a weighted superposition of the supernate TEDE and the sludge-solids TEDE, which conservatively treats the sludge solids as if it has zero volume; i.e.,

\[ TEDE_{slurry} = TEDE_{sup} + C_{solids} \times TEDE_{solids} \]  

where
\[
TEDE_{sup} = \text{unit dose factor for supernate} = 3.34 \times 10^{-3} \text{ rem/gal [Ref. 8]}
\]
\[
TEDE_{solids} = \text{unit dose factor for sludge solids} = 8.61 \times 10^{-4} \text{ rem/g} [\text{Ref. 8}]
\]

and \( C_{solids} \) is the concentration of sludge solids in slurry waste given by:

\[ C_{solids} = \rho_{slurry} \times X_{solids} \left( 3.785 \frac{L}{gal} \right) \left( 1,000 \frac{g}{kg} \right), \text{ in g/gal} \] 

where \( X_{solids} \) is the sludge solids mass fraction for the waste slurry.

During a deflagration event, the aerosol generation mechanism is associated with the bubble entrainment caused by the radiative heat transfer at the liquid surface. With the supernate on top of the sludge (and saltcake), it is reasonable to expect the aerosolization of the “Mass-at-Risk” (MAR) is mostly a surface phenomenon with the sludge solids in the bottom undisturbed. As a result, the source term is expected to be composed of supernate with very little sludge solids. When detonation occurs, sludge solids below the supernate could potentially be disturbed by pressure shock wave. However, it is not expected that the disturbed solids would reach the surface of the supernate to become aerosolized. It is known that the passage of the pressure shock wave could take place in the order of milliseconds and the sludge solids would have to rise tens of inches to the surface to be aerosolized. Reference 9 shows the vertical velocity of the trapped hydrogen after a seismic event occurs is approximately 0.1 ft/sec. Knowing that sludge particles are much heavier than hydrogen, the rise velocity of the sludge solids would be even slower. Therefore, it is again reasonable to expect that the slurry actually aerosolized during a detonation event contains very little sludge solids.

Based on the aforementioned argument, it is justifiable to use a 0\% for the sludge solids concentration \( X_{solids} \). For conservatism, this analysis assumes the value of 1\% for \( X_{solids} \) which also corresponds to an IDP of 9.8 \times 10^7 \text{ rem/gal} [\text{Ref. 2}]. With \( X_{solids} \) determined, the slurry density is given by the following relationship:
\[ \rho_{\text{slurry}} = \frac{1}{\frac{X_{\text{solids}}}{\rho_{\text{solids}}} + \frac{1 - X_{\text{solids}}}{\rho_{\text{sup}}}} \]  

(17)

Where

\( \rho_{\text{solids}} \) = sludge solids density = 5 kg/L \ [Ref. 3]  
\( \rho_{\text{sup}} \) = supernate density = 1.6 kg/L \ [Ref. 3]

Results of Analysis

With the methodology described, this analysis evaluates the hydrogen concentration in the tank vapor space and the consequence parametrically as a function of the liquid level. The results of the calculation are shown in Figures 1 and 2.

Figure 1. Hydrogen Vapor Space Concentration Versus Fill Conditions
From Figure 1, it can be seen that the hydrogen concentration increases with the liquid level and the increase becomes especially pronounced when the level passes ~300 inches. This is because the liquid level is beginning to approach the top of the tank and the vapor space is decreasing rapidly. Figure 1 also shows that Scenario B tends to yield slightly higher hydrogen concentration. This is due to the higher void fraction and relative release fraction of the trapped hydrogen in saltcake.

On the other hand, Figure 2 shows that the offsite dose stays relatively constant (around 0.05 rem), for liquid levels up to about 288 inches. In this range, the hydrogen concentration is below 12% and the combustion is manifested in the form of deflagration. In fact, the offsite dose actually decreases slightly with the liquid level because the increase in the hydrogen concentration is not sufficient to offset the decrease of the vapor space volume. From Figure 2, it can also be seen that the offsite doses for both Scenario A and Scenario B experience sudden jumps at liquid level around 320 inches. This is the result of the transition from deflagration to detonation when the hydrogen concentration reaches 12%. For Scenarios A and B, the maximum offsite dose are 2.1 rem and 1.9 rem, respectively. The reason for the higher dose of Scenario A is because it reaches the LEL earlier so that it has a slightly larger vapor space volume than that of Scenario B.
Conclusion

The present study has shown that the explosion at the CST Facility can be reasonably represented by the two bounding scenarios of different configurations. It has been found that the mitigated consequence to the offsite receptor for a bounding CST tank following a seismic event is 2.1 rem; with 40 inches of saltcake in the bottom, 50 inches of settled sludge, and 235 inches of supernate on the top. The reason for higher consequence for the configuration is the higher void fraction and release fraction in the saltcake.

References:

1. “Waste Characterization System,” WG 17/WCS 1.5PROD/WCS 1.5, March 2011 (selected data summarized in e-mail attachment of Appendix B of Ref. 2).