

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U. S. Department of Energy.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Potential Flammable Gas Explosion in the TRU Vent and Purge Machine

M. R. Yeung, WSMS
J. Norkus, Parallax
S. J. Mentrup, WSRC
M. K. Gupta, WSMS

Abstract

The objective of the analysis was to determine the failure of the Vent and Purge (V&P) Machine due to potential explosion in the Transuranic (TRU) drum during its venting and/or subsequent explosion in the V&P machine from the flammable gases (e.g., hydrogen and Volatile Organic Compounds [VOCs]) vented into the V&P machine from the TRU drum. The analysis considers: a) increase in the pressure in the V&P cabinet from the original deflagration in the TRU drum including lid ejection, b) pressure wave impact from TRU drum failure, and c) secondary burns or deflagrations resulting from excess, unburned gases in the cabinet area. A variety of cases were considered that maximized the pressure produced in the V&P cabinet. Also, cases were analyzed that maximized the shock wave pressure in the cabinet from TRU drum failure. The calculations were performed for various initial drum pressures (e.g., 1.5 and 6 psig) for 55 gallon TRU drum. The calculated peak cabinet pressures ranged from 16 psig to 50 psig for various flammable gas compositions. The blast on top of cabinet and in outlet duct ranged from 50 psig to 63 psig and 12 psig to 16 psig, respectively, for various flammable gas compositions. The failure pressures of the cabinet and the ducts calculated by structural analysis were higher than the pressure calculated from potential flammable gas deflagrations, thus, assuring that V&P cabinet would not fail during this event. National Fire Protection Association (NFPA) 68 calculations showed that for a failure pressure of 20 psig, the available vent area in the V&P cabinet is 1.7 to 2.6 times the required vent area depending on whether hydrogen or VOCs burn in the V&P cabinet. This analysis methodology could be used to design the process equipment needed for venting TRU waste containers at other sites across the Department of Energy (DOE) Complex.

Introduction

The V&P cabinet is a rectangular box structure which is intended to enclose either a 55 gallon drum or other container during the performance of a remote drum venting operation as shown in Figure 1. A small single – station glovebox is attached to the top of the cabinet and a mounting plate is used to seal both the top of the cabinet and the bottom of the glovebox. This mounting plate will also support the mechanical device which controls the drum operation. The interior volume of the Vent and Purge Machine is 76.85 ft³ (2.18 m³). The length and width are 4.83 feet and 2.92 feet, respectively. A dedicated air flow system is connected to the cabinet to ensure constant air flow and a negative pressure environment. This cabinet is designed to include a 24

inch by 24 inch square High Efficiency Particulate Air (HEPA) filter housing on one side and a connection for ventilation exhaust duct work (21.75 inches by 21.75 inches) on the other. The air handling system is capable of generating up to -9.5 inches of water column at stall conditions. The cabinet is capable of sustaining internal negative pressure in excess of this level without damage. Two doors are present in the cabinet. One is a large access door, which has been sized to permit the insertion and retrieval of a drum which is supported by a drum dolly. The second door is a small access door used primarily to inspect the top surface of the drum for contaminants prior to opening the large access door. The distance from the top of the drum to the cabinet top is 20 inches. The distance from the top of the drum to the outlet of the ventilation transition piece is 34.6 inches.



Figure 1 Purge and Vent Cabinet.

The maximum initial pressure in the waste drum is either 1.5 psig or 6 psig. The purpose of this analysis is to determine the potential pressures arising from a deflagration in a TRU waste drum while inside the V&P machine. Deflagrations have previously been analyzed for up to 12% hydrogen and stoichiometric toluene concentrations within the waste drums¹. However, sampling of un-vented drums has revealed hydrogen concentrations above 12% (maximum 64% hydrogen) and VOC at very high levels. This has the potential to challenge the previous analysis in the following manner:

1. Increase in the pressure resulting from the original deflagration including lid ejection
2. Pressure wave impact from drum failure

3. Secondary burns or deflagration resulting from excess, unburned combustion gases in the cabinet area

Therefore, a set of cases were developed, as shown in Table 1, to bound these three issues for both elevated hydrogen and VOCs.

Table 1 Cases Analyzed.

Case number	Description	Drum conditions	Function
1a	Determine the maximum pressure in the cabinet from the stoichiometric hydrogen deflagration in the drum	Stoichiometric hydrogen (29.6 %)	Provide the highest deflagration pressure in the drum for hydrogen and the maximum pressure inside the cabinet for cases in which the drum does not fail, but merely vents to the cabinet.
1b	Determine the maximum pressure in the cabinet from the stoichiometric toluene deflagration in the drum.	Stoichiometric toluene (2.27%)	Provide the highest deflagration pressure in the drum for VOCs and the maximum pressure inside the cabinet for cases in which the drum does not fail, but merely vents to the cabinet.
2a	Determine the shock pressure from drum failure resulting from stoichiometric hydrogen deflagration in drum upon cabinet top.	Stoichiometric hydrogen (29.6 %)	Maximize the shock wave pressure from the drum failure and/or hydrogen deflagration on the cabinet top assuming that the drum lifts off.
2b	Determine the shock pressure from the drum failure resulting from the stoichiometric toluene deflagration in the drum.	Stoichiometric toluene (2.27%)	Maximize the shock wave pressure from the drum failure/toluene deflagration on the cabinet top assuming that the drum lifts off.
3a	Determine the maximum pressure in the cabinet from 70% hydrogen deflagration in the drum. Since this condition is “fuel rich,” there will be excess fuel and the potential for secondary deflagrations in the cabinet once the drum fails and vents to the cabinet.	70% hydrogen	Maximize the pressure in the cabinet for the secondary deflagration. The concentration chosen bounds the maximum hydrogen concentration seen in the TRU drums and is below the upper flammability limit.
3b	Determine the maximum pressure in the cabinet from 31% hydrogen/4.04% toluene deflagration in the drum. Since this condition is “fuel rich,” there will be excess fuel and the potential for secondary deflagrations in the cabinet once the drum fails and vents to the cabinet.	31% hydrogen, 4.04 % toluene	Maximize the pressure in the cabinet for a secondary deflagration. The VOC concentration (toluene) was fixed and the hydrogen concentration was set to the point at which the mixture equals the upper mixture

Case number	Description	Drum conditions	Function
			flammability limit.

Input Data

Table 2 lists the drum physical dimensions and assumed initial conditions used in the analysis. The inputs in Table 2 are used to calculate the deflagration pressures for the different types of VOCs that are found inside the TRU drums.

Table 2 Base Input Items.

Input Item	Value
Inner diameter of vented TRU drum ²	22.5 inches
Inner usable height of 208L vented TRU drum ²	32.0 inches
Initial pressure	1.5 or 6 psig
Drum Void Fraction	0.75
Oxygen concentration in air	21%
Hydrogen combustion energy ³	57.8 kcal/mole
Toluene combustion energy ³	901.5 kcal/mole

Analytical Models

The methods used to analyze each case are treated in a piecewise manner.

For Case 1 (a-stoichiometric hydrogen [29.6%]; b-stoichiometric toluene [2.27%]), the resulting AICC deflagration pressures within the drum are calculated using the methodology described in Reference 4. The product gases are then expanded isentropically into the entire cabinet volume. The final cabinet pressure is determined from this expansion. This is the method employed in the previous calculation for deflagration pressures and venting to the V&P cabinet contained in References 5 and 6. The major differences between the analysis is the use of stoichiometric hydrogen instead of 12% hydrogen, a larger cabinet volume (approximately 10 times the drum volume versus 2 times) and a higher drum initial pressure.

For Case 2 (calculation of the shock wave pressure from drum failure), the peak drum pressure from the deflagrations calculated in Case 1 is used to calculate the energy and pressure in the shock wave as described in Isentropic Expansion.

For Case 3 (a-70% hydrogen; b-31% hydrogen; 4.04% toluene), the initial conditions were selected to generate the maximum pressure in a secondary deflagration that would occur in the cabinet following the drum deflagration. In this scenario, the following sequence of events occurs:

1. The TRU drum deflagrates and pressurizes.
2. The pressure is sufficient to fail the lid and vent the gases to the cabinet.
3. The cabinet is pressurized. The pressure is calculated the same way as the isentropic expansion in Case 1.

4. Since the flammable vapors were above the stoichiometric limit in the drum, the vented gases will become combustible in the cabinet.
5. A secondary deflagration occurs in the cabinet which is initiated at an elevated pressure.
6. The deflagration vents through both the inlet and the outlet ducts from the cabinet.

This is the most challenging of the scenarios. Portions 1-4 will be treated very similarly to the process in Case 1. However, the peak pressure resulting from the secondary deflagration in the cabinet with gas venting will be calculated using the NFPA methodology for explosion vent design. This is a very conservative approach. The NFPA vent design methodology assumes that the worst case explosion conditions are present (stoichiometric) for a given flammable gas. When the gases from the drum are vented to the cabinet and completely mix (Case 3a), the hydrogen is just above the flammability limit, and for Case 3b, the toluene/hydrogen mixture is below the composite lower flammability limit. However, since from the point of venting to complete mixing in the cabinet, the gases will be flammable and it is assumed that a burn occurs.

ISENTROPIC EXPANSION

The pressure which would result from the expansion of the product gas mixture inside the drum into the interior of the venting chamber is modeled by assuming isentropic expansion of the product gas cloud from the adiabatic isobaric complete combustion temperature in the drum to equilibrium with the remainder of the cabinet atmosphere.

Based on the ideal gas law, the volume of the product gas after the isentropic expansion can be written as:

$$V_{h,f} = V_{h,i} \left(\frac{P_{h,i}}{P_{h,f}} \right) \left(\frac{T_{h,f}}{T_{h,i}} \right) \left(\frac{n_{h,f}}{n_{h,i}} \right) \quad (1)$$

where:

- V = Volume,
- P = Pressure (absolute),
- T = Temperature (absolute),
- n = Number gas moles.

The 'i' and 'f' subscripts denote initial and final states, respectively, and the 'h' subscript denotes the hot product gas cloud. The initial temperature and pressure are assumed to be those assumed for the drum (T_i and P_i) before the deflagration and the initial volume is the drum gas volume. The final to initial gas mole ratio is simply the product to reactant gas mole ratio (N_p/N_r) which is set to unity since this factor has already been accounted in the AICC pressure calculations. The final temperature is that for adiabatic isobaric complete combustion ($T_{p=c}$) corrected for isentropic compression to the actual final pressure, as shown below:

$$T_{h,f} = T_{p=c} \left(\frac{P_f}{P_i} \right)^{\frac{k-1}{k}} \quad (2)$$

where: k = Specific heat ratio ($k = C_p/C_v$),
 C_p = Specific heat at constant pressure,
 C_v = Specific heat at constant volume ($C_v = C_p - R$), and
 R = Universal gas constant.

Note that P_i appears in the dominator since the isobaric conditions are assumed to exist during the deflagration. Combining eqns. (1) and (2) gives a final hot gas volume of:

$$V_{h,f} = V_{h,i} \left(\frac{T_{p=c}}{T_i} \right) \left(\frac{P_f}{P_i} \right)^{\frac{k-1}{k}} \left(\frac{P_i}{P_f} \right) \left(\frac{N_p}{N_r} \right) = V_{h,i} \left(\frac{T_{p=c}}{T_i} \right) \left(\frac{P_i}{P_f} \right)^{1/k} \left(\frac{N_p}{N_r} \right) \quad (3)$$

The initial cold gas volume is that in the venting chamber outside the drum. The final cold gas volume after isentropic compression can be written as:

$$V_{c,f} = V_{c,i} \left(\frac{P_i}{P_f} \right)^{1/k} \quad (4)$$

The total volume (V_T) is the sum of the hot and cold gas volumes [eqns. (3) & (4)]:

$$V_T = \left[V_{c,i} + V_{h,i} \left(\frac{T_{p=c}}{T_i} \right) \left(\frac{N_p}{N_r} \right) \right] \left(\frac{P_i}{P_f} \right)^{1/k} \quad (4a)$$

Note that a single value for the specific heat ratio has been assumed, which implies that a value averaged to reflect the properties of both the hot product gas and the cold gas in the venting chamber. The final to initial gas pressure ratio is therefore given by the following expression:

$$\frac{P_f}{P_i} = \left[\frac{V_{c,i} + V_{h,i} \left(\frac{T_{p=c}}{T_i} \right) \left(\frac{N_p}{N_r} \right)}{V_T} \right]^k \quad (5)$$

which can also be written as:

$$\frac{P_f}{P_i} = \left\{ 1 + \frac{V_{h,i}}{V_T} \left[\left(\frac{T_{p=c}}{T_i} \right) \left(\frac{N_p}{N_r} \right) - 1 \right] \right\}^k \quad (5)$$

BLAST WAVE PRESSURE

The energy associated with the blast wave resulting from the failure of the drum lid can be represented by the following equation ⁷:

$$W = E_w \frac{(P_2 - P_1)v_0}{k - 1} \quad (6)$$

Where k is the ratio of specific heats (1.4); v₀ refers to the volume of the gas at pressure P₂, P₂ is the burst pressure and P₁ is the atmospheric pressure. Also, the energy of the wave is 40% of the total (E_w) if there is ejection of a major vessel section, such as the drum lid ⁷.

The characteristics of the blast wave produced by a deflagration are generally determined by application of scaling laws. One technique is the TNT equivalent method in which the deflagration energy and the distance to the target are scaled according to:

$$z = \frac{r}{W_{TNT}^{1/3}} \quad (7)$$

Where ‘r’ is the distance to the target from the deflagration and W_{TNT} is the mass of the explosive in pounds of TNT, and ‘z’ is the scaled distance. The deflagration energy must be translated into mass of TNT. The TNT specific energy (E_{TNT}) is 4.52 MJ/kg (1.515x10⁶ ft-lb_{s_f}/lb_m TNT).

$$W_{TNT} = \frac{W}{E_{TNT}} \quad (8)$$

To determine the peak overpressure associated with the wave, use Figure 17.5a from Reference 7. This correlation is usually applied for an open air explosions modeling a supersonic phenomena. It is applied for a deflagration condition in the cabinet which is a subsonic phenomena where the conditions present in the supersonic phenomena (e.g. reflected pressure) are not significant.

DEFLAGRATION VENTING

NFPA 68 **Guide for Venting of Deflagrations**, Section 6.3, Venting of Gas or Mist Deflagration in High-Strength Enclosures ⁸ provides a method for calculating the required vent area in order to prevent structural failure. This method can also be applied to calculate the worst peak pressure given the available vent area. The V&P cabinet is classified as a high strength enclosure since the failure pressure is above 1.5 psig per NFPA 68.

The length-to-diameter ratio (L/D), of the enclosure determines the equation(s) that is to be used for calculating the necessary vent area. For noncircular enclosures, the value that is to be used for diameter is the equivalent diameter given by the following equation:

$$D = 2 \left(\frac{A^*}{\pi} \right)^{1/2} \quad (9)$$

where:

D = equivalent diameter

A* = cross-sectional area normal to the longitudinal axis of the space

For the cabinet, A* is calculated as 14.1 ft² (LxW=4.83 ft x 2.92 ft) and D as 4.24 feet. The resulting L/D ratio is 1.14 and this approach applies. For L/D values of 2 or less, the following equation is used for calculating the necessary vent area, A_v, in m² for an allowable pressure, P_{red} is:

$$A_v = \left[(0.127 \log_{10} K_G - 0.0567) P_{red}^{-0.582} + 0.175 P_{red}^{-0.572} (P_{stat} - 0.1) \right] V^{\frac{2}{3}} \quad (10)$$

where:

A_v = vent area (m²)

K_G ≤ 550 bar-m/sec

P_{red} ≤ 2 bar and at least 0.05 bar > P_{stat} (Maximum allowable pressure)

P_{stat} ≤ 0.5 bar (vent opening pressure)

V = enclosure volume (m³)

In this case, instead of calculating the vent area, the worst case maximum peak pressure is calculated. P_{stat}, the vent opening pressure is taken as 0 psig (0 bar) since there are no dampers preventing the escape of gases from the cabinet. For hydrogen and toluene, the values of K_G are 550 bar-m/s and 94 bar-m/sec, respectively (Table D.1⁸).

Since the deflagration in the cabinet vapor space occurs at an elevated pressure, a correction factor must be applied. For a given vent size, the maximum pressure that develops during the venting of a deflagration (P_{red}) varies as a function of the initial absolute pressure raised to an exponential power, γ. For this calculation, the ratio of the absolute pressure when the vent closure opens to the absolute pressure at the time is assumed to be constant. The recommended values of the exponent varies inversely with the ratio of the vent area, A_v to the 2/3 power of the enclosure volume, V; that is, γ varies inversely with A_v/V^{2/3}. The new P_{red,2} pressure is calculated as follows:

$$P_{red,2} = (P_{red,1}) \left(\frac{P_2}{P_1} \right)^\gamma \quad (11)$$

Where

P_{red,2} = Actual maximum pressure (bar abs) developed by the deflagration in a vented enclosure when the initial elevated pressure before ignition is P₂ (bar abs)

P_{red,1} = P_{red} as determined converted to bar, abs

P₂ = Elevated initial pressure before ignition (bar abs). This is determined by the

output of the isobaric expansion calculation.

$$P_1 = \text{Atmospheric pressure, 1.0 bar abs}$$

It should be noted that this pressure is the worst deflagration pressure which can develop in the cabinet. For the secondary deflagrations evaluated in this calculation, Case 3a (hydrogen) is barely over the lower flammability limit when mixed in the cabinet volume and for Case 3b (hydrogen/toluene), the mixture is below the composite lower flammability limit. Both of these cases are far away from stoichiometric conditions and would not be expected to develop the pressures calculated in this analysis. Therefore, for Case 3a, the K_G used is for hydrogen and for Case 3b the K_G used is for toluene, since these are the species which dominate the secondary deflagrations for these events.

Results

The following Tables 3 and 4 contain the results of the cases considered.

Table 3 Results for Various Cases for an Initial Pressure 1.5 psig in TRU Drum.

Case	Flammable concentrations	Scenario	Pressure	Capacity of cabinet components
Case 1a Leak Pressure H2	Stoichiometric hydrogen in the drum (29.7 %)	Complete combustion of hydrogen in the drum. No catastrophic failure of the lid. The combustion products escape from drum and expand into the cabinet area. No venting from the cabinet is assumed.	Peak cabinet pressure: 16.2 psig	Cabinet - 100 psig
Case 1b Leak Pressure VOC	Stoichiometric toluene in the drum (2.27 %)	Complete combustion of toluene in the drum. No catastrophic failure of the lid. The combustion products escape from the drum and expand into the cabinet area. No venting from the cabinet is assumed.	Peak cabinet pressure: 16.0 psig	Cabinet - 100 psig
Case 2a – Pressure Wave	Stoichiometric hydrogen in the drum (29.7 %)	Complete combustion of hydrogen in the drum. The drum lid fails catastrophically (lifts). The blast wave impacts the top of the cabinet.	The blast pressure on the top of the cabinet: 50 psig The blast pressure in the outlet duct: 12 psig	Cabinet - 100 psig Outlet duct shell – 80 psig
Case 2b – Pressure Wave VOC	Stoichiometric toluene in the drum (2.27 %)	Complete combustion of toluene in the drum. The drum lid fails catastrophically (lifts). The blast wave impacts the top of the	The blast pressure on top of the cabinet: 55 psig	Cabinet - 100 psig Outlet duct shell – 80 psig

Case	Flammable concentrations	Scenario	Pressure	Capacity of cabinet components
		cabinet	The blast pressure in the outlet duct: 15 psig	
Case 3a – Continuing Deflagration	70% hydrogen	Partial combustion of hydrogen in the drum. The lid fails (Note: energy from hyper-stoichiometric deflagration is lower than the stoichiometric condition in Case 2.). The combustion products and uncombusted hydrogen vent to the cabinet and pressurize the cabinet. A secondary deflagration occurs. The combustion products vent from the cabinet reducing the peak deflagration pressure.	Peak cabinet pressure: 48.4 psig (inlet vent only) 23.1 psig (inlet and outlet vent)	Inlet Filter Housing Bolts – 54 psig Filter Train bolts – 21 psig
Case 3b- Continuing Deflagration VOC	31% hydrogen, 4.04 % toluene	Partial combustion of hydrogen in the drum. The lid fails (Note: the energy from hyper-stoichiometric deflagration is lower than the stoichiometric condition in Case 2). The combustion products and uncombusted hydrogen and toluene vent to the cabinet and pressurize the cabinet. A secondary deflagration occurs. The combustion products vent from the cabinet reducing the peak deflagration pressure.	Peak cabinet pressure: Venting conditions based on toluene: 49.6 psig (inlet vent) 26.8 psig (inlet and outlet vent)	Inlet Filter Housing Bolts – 54 psig Filter Train bolts – 21 psig .

Table 4 Results for Various Cases for an Initial Pressure 6 psig in TRU Drum.

Case	Flammable concentrations	Scenario	Pressure	Notes
Case 1a Leak Pressure H2	Stoichiometric hydrogen in the drum (29.7 %)	Complete combustion of hydrogen in the drum. No catastrophic failure of the lid. The combustion products escape from the drum and expand into the cabinet area. No venting from the cabinet is assumed.	Peak cabinet pressure: 24.7 psig	Cabinet - 100 psig
Case 1b Leak Pressure VOC	Stoichiometric toluene in the drum (2.27 %)	Complete combustion of toluene in the drum. No catastrophic failure of the lid. The combustion products escape from the drum and expand into the cabinet area. No venting from the cabinet is	Peak cabinet pressure: 24.5 psig	Cabinet - 100 psig

Case	Flammable concentrations	Scenario	Pressure	Notes
		assumed.		
Case 2a – Pressure Wave	Stoichiometric hydrogen in the drum (29.7 %)	Complete combustion of hydrogen in the drum. The drum lid fails catastrophically (lifts). The blast wave impacts top of the cabinet.	The blast pressure on top of the cabinet: 50 psig Blast pressure in the outlet duct: 14 psig	Cabinet - 100 psig Outlet duct shell – 80 psig
Case 2b – Pressure Wave VOC	Stoichiometric toluene in the drum (2.27 %)	Complete combustion of toluene in the drum. The drum lid fails catastrophically (lifts). The blast wave impacts top of the cabinet	The blast pressure on top of the cabinet: 55 psig Blast pressure in outlet duct: 16 psig	Cabinet - 100 psig Outlet duct shell – 80 psig
Case 3a – Continuing Deflagration	70% hydrogen	Partial combustion of hydrogen in the drum. The lid fails (Note: energy from hyper-stoichiometric deflagration is lower than the stoichiometric condition in Case 2). The combustion products and uncombusted hydrogen vent to the cabinet and pressurize the cabinet. A secondary deflagration occurs. The combustion products vent from the cabinet reducing the peak deflagration pressure.	Peak cabinet pressure: 63.2 psig (inlet vent only) 31.4 psig (inlet and outlet vent)	Inlet Filter Housing Bolts – 54 psig Filter Train bolts – 21 psig
Case 3b- Continuing Deflagration VOC	31% hydrogen, 4.04 % toluene	Partial combustion of hydrogen in the drum. The lid fails (Note: energy from hyper-stoichiometric deflagration is lower than stoichiometric condition in Case 2). The combustion products and uncombusted hydrogen and toluene vent to the cabinet and pressurize the cabinet. A secondary deflagration occurs. The combustion products vent from the cabinet reducing the peak deflagration pressure.	Peak cabinet pressure: Venting conditions based on toluene: 74.1 psig (inlet vent) 40.0 psig (inlet and outlet vent)	Inlet Filter Housing Bolts – 54 psig Filter Train bolts – 21 psig

Conclusions

Deflagration pressures have been calculated for the flammability conditions which will most severely challenge the V&P cabinet and ductwork. It is shown that the V&P cabinet would not fail except for the filter train bolts for the hyper-stoichiometric conditions in the drum for both the initial pressures. If conservatism in the analysis are considered then the V&P cabinet would survive the deflagration event.

Conservatism

In addition to the main conclusions, several conservatisms were identified in the analysis, and these are described below.

1. **AICC Pressure Calculations** — The pressure calculations performed in this analysis for combustion of flammables assume an adiabatic isochoric complete combustion of the flammable mixture. Normally, the combustion is not 100% efficient and there could be significant heat losses to the surrounding surfaces during the combustion process. The Bureau of Mines Bulletin #680 reports a peak pressure of 108 psig from the combustion of a stoichiometric mixture of methane and air. The AICC pressure calculated in Reference 9 is 162 psig. This shows that idealized combustion of methane achieves only 66% of the pressure calculated by AICC method or, in other words, the actual pressure in the drum would be about 34% lower than what is calculated in this analysis for VOCs.
2. **Flammable Vapors in Drum** — It is assumed for the bounding case that the flammable vapors are at composite upper flammability limit. The drums that are at this condition are difficult to ignite.
3. **Pressure Calculation during Venting of Gases** — NFPA 68 guidance is used for calculating the pressure during venting of gases from a secondary deflagration in the V&P cabinet. The NFPA pressure calculation methodology uses a stoichiometric mixture of flammables. It does not provide any guidance if the flammables are below the stoichiometric values. The flammable vapor concentration in the V&P cabinet is slightly higher than lower flammability limit (assuming a homogeneous mixture) for the secondary deflagration. Thus, the use of NFPA pressure calculation methodology for a stoichiometric mixture provides very conservative final pressure in the V&P cabinet.
4. **Final Pressure Calculation in the V&P Cabinet during Secondary Deflagration** — It is assumed that there is no venting of gases released into the V&P cabinet from the deflagration (that results in the lid failure, i.e., Cases 3a and 3b) in the drum. The resulting pressure (this pressure is significantly higher than atmospheric pressure) from this release of gases is used as an initial pressure for the secondary deflagration and for venting of the gases. Neglecting the venting of gases from the V&P cabinet during first deflagration is conservative.
5. **Combustible Conditions in the Cabinet Following the Drum Deflagration** — It has been assumed that a secondary deflagration in the cabinet could occur for drums which have flammable vapors above the stoichiometric concentrations. However, when the drum vents from the deflagration, the flammable vapors will escape at high pressure and mix with the cabinet vapor space. For a portion of that time, some of the escaping gases will be below the flammability limit, some will be flammable, and some will be flammable but have insufficient oxygen. It is not possible that all of the escaping flammable gases will burn during a secondary cabinet deflagration.
6. **Pressure Time Transient Calculation.** — We have provided the peak pressure that occurs in the V&P cabinet in this analysis. The time it takes to reach that peak pressure and how it decays is not calculated. The peak pressure without a time history is a conservative input to

the structural evaluation. A quantification of the pressure-time history would help in reducing the conservatism in the structural analysis.

7. NFPA 68 Vent Area Design Calculations — NFPA 68 provides a methodology for the design of required vent area in a structure as a function of the failure pressure of that structure from a potential flammable gas deflagration. This NFPA 68 methodology was used to determine the vent area needed in the V&P cabinet as a function of the failure pressure of the V&P cabinet from a potential flammable gas deflagration. The results of this calculation show that for a failure pressure of 20 psig, the available vent area in the V&P cabinet is 1.7 to 2.6 times the vent area required by NFPA 68 calculations depending on whether hydrogen or toluene burns in the V&P cabinet.

Considering the above conservatisms, it is qualitatively judged that the reasonable conservative peak pressure could be 50% below the peak pressures calculated in this analysis.

References

1. Letter from Gordon, R. J. to Garrett, T. P., "Explosion Characteristics of H₂-Air Mixtures Relative to Transuranic (TRU) Waste Containers," E. I. DuPont de Nemours and Company, Savannah River Plant, Aiken, SC, February 16, 1986.
2. Website for DOT-7A containers at http://rampac.com/DOT_7A_Type_A_Documents.htm.
3. Kutchta, J. M. Investigation of Fire and Explosion Accidents in the Chemical, Mining and Fuel-Related Industries - A Manual. Bureau of Mines Bulletin 680, U. S Government Printing Office, Washington, DC, 1985.
4. Thomas, J.K. Combustion, Flame Front Propagation, and Radiative Heat Transfer Models for Deflagrations. WSRC-RD-93-007, Savannah River Site, Aiken, SC, April 1993.
5. B. H. Cleaver. Strategy and Planning for SWMF Upgraded SAR Accident Analysis (U). S-CLC-G-00024, Rev. 0, 4/1/95.
6. J. K. Thomas. TRU Waste Drum Vent and Purge Design Basis Deflagration (U). SRT-LWA-94-0084, May 25, 1994.
7. F. P. Lees. Loss Prevention in the Process Industries, Vol. 1. (Butterworth- Heinemann Ltd, 1980).
8. National Fire Protection Association, **NFPA 68 Guide for Venting of Deflagrations**, 2002 edition.
9. M. R. Yeung. Deflagration Analysis for Type IIIA and IV Tank Underliners (U). S-CLC-F-00428, Rev. 0, 2002.

Bolt