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**PRESSURE RESULTING FROM AN
ITP WASTE TANK DEFLAGRATION (U)**

By

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EXECUTIVE SUMMARY

The SRS waste tanks to be employed with the In-Tank Precipitation (ITP) process are undergoing a structural evaluation in order to define their response to a hypothetical deflagration accident. At the request of the Waste Management and Environmental Remediation Division (WM&ER - High Level Waste Programs), a task was initiated to predict the peak gas pressure which would result from a deflagration (Thomas and Hensel 1993a). This report presents the final results of the deflagration peak gas pressure evaluation.

The DPAC computer code was employed to calculate the pressure which would result from a deflagration in an ITP waste tank. Hydrogen-benzene mixtures with air were evaluated to establish upper-bound deflagration pressures. Best-estimate calculations of the peak deflagration pressure were generated using gas compositions which account for the initial nitrogen inerting, the water vapor content of the air, and oxygen intake due to atmospheric exchange mechanisms. The calculated pressures for the air mixtures are less than 17 psig for both Tank 48 and 49 at a fill level of 1/2. Considering the effects of water vapor, the maximum calculated pressure for the air mixtures is 21 psig and occurs with a stoichiometric air mixture in Tank 48 at a fill level of 1/10. The maximum gas pressure calculated for the best-estimate mixtures is 15.1 psig.

A set of parametric calculations was performed which demonstrated that the calculated peak pressures are not strongly sensitive to variations in the input parameters. Furthermore, the input parameters were selected in a conservative fashion to account for uncertainty in the experimental data. The models employed by DPAC also incorporate a number of implicit conservatisms. As a result, the calculated peak gas pressures are upper-bound values for a given mixture composition. The uncertainty in the pressures is therefore one-sided, and the pressures calculated with true best-estimate input data and models would be lower.

Previous analyses of waste tank deflagration pressures have either neglected significant modes of energy dissipation (venting and radiation) and/or have treated the gas as a single region and therefore underpredicted the energy dissipation rates. Additionally, none of the previous analysis were capable of accurately calculating the burn time, so that the total energy dissipated via venting and radiation could not be accurately calculated. The analysis reported here provides a more accurate evaluation of these energy dissipation modes and, as a result, gives significantly lower peak gas pressures.

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1.0 INTRODUCTION

1.1 Background

The SRS waste tanks to be employed with the In-Tank Precipitation (ITP) process are undergoing a structural evaluation in order to define their response to a hypothetical deflagration accident. At the request of the Waste Management and Environmental Remediation Division (WM&ER - High Level Waste Programs), a task was initiated to predict the peak gas pressure which would result from a deflagration (Thomas and Hensel 1993a). This report presents the final results of the deflagration peak gas pressure evaluation.

The waste tanks of interest in this evaluation are Tanks 48 and 49. These tanks are equipped with a nitrogen purge gas system that removes combustible gases from the tank vapor space and displaces oxygen. The deflagration accident scenario assumes that the purge gas system has failed and that a combustible gas mixture accumulates due to the buildup of combustible gases and inleakage of oxygen. Both hydrogen (H_2) and benzene (C_6H_6) are generated in these tanks as a result of radiolysis (Walker 1993).

1.2 Waste Tank Description

The tanks of interest in this evaluation (48 & 49) are of the Type IIIA design class (SRS 1991). Figure 1 is a cross section of a Type IIIA waste tank. The primary liner has an inside diameter of 85' and a height of 33'; the central column has an outer diameter of 6' 9.5" (SRS 1979). The Type III tanks have an internal volume of approximately 5.2×10^6 liters. The Type III waste tanks employ approximately 4 miles of 2" schedule 40 (O.D. = 2.375") carbon steel coiling coil tubes (SRS 1991). These tubes are suspended from the top of the primary liner and supported at the bottom of the primary liner by u-bends in the tube. The other Type IIIA waste tank design features are not of direct interest in this evaluation.

1.3 Deflagration Pressure Analysis Methodology

The peak gas pressures resulting from a deflagration were calculated using the Deflagration Pressure Analysis Code (DPAC), which was written as part of this task. The code accounts for venting, radiative heat transfer, structural deformation, and gas PdV work, and can model nonstoichiometric mixtures containing excess inert concentrations (N_2 and H_2O). The total gas volume is divided into product and reactant gas control volumes; each control volume is treated as homogeneous and the energy, mass, and state

equations are solved for each volume at each time step. The models employed by DPAC and the code itself were benchmarked against hand calculations and relevant experimental data. The combustion, flame front propagation, and thermal radiation data and models are discussed in Thomas (1993); DPAC and the venting and gas PdV work models are discussed in Hensel (1993).

2.0 DESCRIPTION OF INPUT DATA

2.1 Gas Compositions

Two classes of gas compositions were considered in this evaluation. The first class is mixtures of combustible gases with dry air containing no excess N_2 ; since this neglects residual N_2 from the ventilation system and water vapor in the air, it is an upper bound with respect to the pressure resulting from a deflagration. Hydrogen-benzene ratios of 60/40 (Tank 49) and 40/60 (Tank 48) were selected as average conditions based on Walker's (1993) gas composition analysis. The second class is the best-estimate mixtures calculated by Morin (1993) which consider the effects of the initial N_2 purge gas and water vapor in the air. The gas compositions reported by Morin are calculated assuming inleakage of air due to atmospheric exchange mechanisms after a loss of ventilation and hence are much more realistic than the air-mixture class. The composition data for these mixture classes are discussed below. Other combustible components, such as isopropanol and methanol, may also be present in the vapor space of the ITP waste tanks (Walker 1993); however, the concentration of these additional components would be sufficiently low that they may be neglected without introducing significant error.

2.1.1 Air Mixture Compositions

Combustible gas concentrations between the lower flammability limit (LFL) and stoichiometric value were examined for the air mixtures. The LFL for a mixture of H_2 and C_6H_6 can be calculated as (Jacobs 1988):

$$LFL = 0.03799 \cdot y_c(H_2) + 0.01198 \cdot y_c(C_6H_6) \quad (1)$$

where: $y_c(H_2)$ = Fraction of H_2 in combustible gas, and
 $y_c(C_6H_6)$ = Fraction of C_6H_6 in combustible gas ($\sum y_c = 1$).

The LFL for H_2 / C_6H_6 ratios of 60/40 and 40/60 calculated using this expression are 2.76% and 2.24%. The stoichiometric combustible concentration for an air mixture is given as:

$$y_{comb} = \frac{1}{1 + [(0.5) y_c(H_2) + (7.5) y_c(C_6H_6)] (1 + R_n)} \quad (2)$$

where: y_{comb} = Combustible gas mole fraction in the reactant mixture, and
 R_n = Ratio of nitrogen to oxygen in air (= 79/21).

The stoichiometric H_2 and C_6H_6 concentrations for an air mixture are 3.59% H_2 and 2.39% C_6H_6 for the 60/40 mixture and 1.71% H_2 and 2.57% C_6H_6 for the 40/60 mixture.

These LFL and stoichiometric compositions are given in Table 1. The pressure resulting from a deflagration was analyzed for 5 compositions between LFL and stoichiometric for half-filled tanks, and for the LFL and stoichiometric compositions for the 1/10 and 3/4 fill levels. For Tank 48 with a 1/10 fill level, intermediate compositions between the LFL and stoichiometric values were also examined since this tank-fill level combination gave the highest pressures. In addition, the water vapor content of the air was considered for a stoichiometric mixture in Tank 48 at a 1/10 fill level (Case 19a); the water vapor content of the air was taken to be 90% of the saturation condition (Morin 1993). Tank fill levels are discussed in Section 2.6.

2.1.2 Best-Estimate Gas Compositions

The time vs. composition calculations of Morin (1993) were employed directly in this evaluation. Figure 2 shows the gas composition for tank 49 following a loss of ventilation for a fill level of 50% at an initial temperature of 40°C with a H₂/C₆H₆ ratio of 60/40. Figure 3 shows the gas composition for tank 48 following a loss of ventilation for a fill level of 135,000 gallons ($\approx$ 10%) at an initial temperature of 40°C with a H₂/C₆H₆ ratio of 40/60. Figure 4 gives the gas composition for tank 48 assuming a temperature of 60°C and that the loss of ventilation occurs simultaneously with the peak in the C₆H₆ generation rate accompanying washing. The LFL [eqn. (1)] and stoichiometric combustible gas concentrations are also shown in these figures. The stoichiometric combustible concentration is given as:

$$y_{\text{comb}} = \frac{y_O}{(0.5) y_c(\text{H}_2) + (7.5) y_c(\text{C}_6\text{H}_6)} \quad (3)$$

where y_O is the oxygen mole fraction in the reactant gas. The stoichiometric gas combustible concentration increases with time due to the increase in oxygen concentration. The combustible gas concentration for these mixtures are below the LFL for some period of time after the loss of ventilation occurs and are hyperstoichiometric after the LFL is reached. The gas pressures given in Section 3 were calculated without consideration of the LFL; similarly, the upper flammability limit (UFL) and minimum oxygen concentrations (MOC) were not considered. That is, the mixture was assumed to combust completely (consuming all of the fuel in hypostoichiometric mixtures and all of the oxygen in hyperstoichiometric mixtures) even if the mixture could not combust. Gas compositions corresponding to Figures 2 through 4 are given in Table 2. The LFL and y_{comb} values, the ratio of the combustible gas concentration to these values, and the ratio of the oxygen to

the total noncombustible gas concentration [e.g. $O_2 / (O_2 + N_2 + H_2O)$] in the reactant gas mixture are also given in Table 2.

2.2 Laminar Flame Speeds

The laminar flame speeds for mixtures of H_2 and C_6H_6 with air at various $O_2/(O_2 + N_2)$ ratios for combustible gas concentrations between the LFL and UFL are shown in Figures 5 (Lewis and Von Elbe 1961) and 6 (Golovina and Fyodorov 1957). The stoichiometric and peak flame speeds shown in these curves are in good agreement with other literature data for H_2 (Coward 1950, Fenn and Calcote 1952) and C_6H_6 (Fenn and Calcote 1952, Heimel and Weast 1957). No data was found for the flame speeds of C_6H_6 - H_2 -air mixtures. Flame speed data for propane-hydrogen-air mixtures with H_2 combustible gas fractions up to 30% are given in Figure 7 (Leason 1953). Since propane (C_3H_8) and C_6H_6 -air mixtures have similar flame speeds and the H_2 -air mixture flame speeds are much larger, it is reasonable to expect that the flame speeds of C_6H_6 - H_2 -air and C_3H_8 - H_2 -air mixtures will exhibit a similar dependence on H_2 concentration. The energy released from C_6H_6 and C_3H_8 combustion, expressed on a per unit mole of oxygen basis, are also similar while that for H_2 is significantly higher (see Appendix A).

The harmonic and arithmetic means were both examined as possible methods to estimate laminar flame speeds for H_2 - C_6H_6 -air mixtures. The harmonic mean flame speed for the mixture may be written as:

$$R_{v,l}(\text{mix}) = \frac{1}{\frac{y_c(H_2)}{R_{v,l}(H_2)} + \frac{y_c(C_6H_6)}{R_{v,l}(C_6H_6)}} \quad (4)$$

where: $R_{v,l}$ = Laminar flame speed (volumetric combustion rate per unit flame front area).

The harmonic mean is equivalent to Le Chatelier's law, which is used to estimate the flammability limits for combustible gas mixtures (Zabetakis 1965). The arithmetic mean of the component flame speeds is calculated as:

$$R_{v,l}(\text{mix}) = y_c(H_2)R_{v,l}(H_2) + y_c(C_6H_6)R_{v,l}(C_6H_6) \quad (5)$$

The peak H_2 -air and C_3H_8 -air flame speeds are approximately 270 and 35 cm/s (Lewis and Von Elbe 1961 and Leason 1953). Equations (4) and (5) give peak flame speeds of 47 and 106 cm/s for a 30% H_2 -70% C_3H_8 mixture using these values, while the data shown in Figure 7 shows a peak flame speed of 40 cm/s for this mixture. The harmonic mean

therefore gives more realistic values, while still being slightly conservative. On this basis, the harmonic mean [eqn. (4)] was employed to calculate the laminar flame speeds for the C_6H_6 - H_2 -air mixtures in this evaluation. Note that, as shown in Figure 7, the increase in flame speed due to the H_2 addition is not sensitive to the mixture stoichiometry.

The flame speed data discussed above are for reactant gas mixtures at 25°C and 1 atmosphere, and it was assumed in this analysis that the volumetric combustion rate per unit surface area was a constant independent of temperature and pressure. In a waste tank deflagration, combustion would occur at progressively higher temperatures and pressures as the remaining reactant gas is pressurized and heated due to expansion of the product gas. Combustible gas-air mixture flame speeds generally decrease with increasing pressure (Egerton and Sen 1952, Lewis and Von Elbe 1961) and increase with increasing temperature. Considering C_6H_6 -air mixtures as an example, Egerton and Sen (1952) cite data showing a flame speed dependence on gas pressure of $P_g^{-1/3}$ and Heimel and Weast (1957) give data showing that flame speed increases for initial gas temperatures from 298 to 700 K over a range of stoichiometric conditions. The effects of increasing reactant gas pressure and temperature will therefore offset to some degree; the net effect could not be determined on the basis of the data examined in this evaluation. However, given the good agreement between the burn times calculated using the methodology employed in DPAC and the experimental results for adiabatic closed vessel combustion of stoichiometric H_2 -air and C_6H_6 -air mixtures (Thomas 1993), the net variation in flame speeds for these mixtures cannot be large.

2.2.1 Air Mixture Compositions

The LFL and stoichiometric laminar flame speeds for air mixtures taken from Figures 5 and 6 are 50 and 190 cm/s (1.6 and 6.2 ft/s) for H_2 and 10 and 45 cm/s (0.33 and 1.5 ft/s) for C_6H_6 ; note that Figure 5 provides only limited data for hypostoichiometric mixtures, and the LFL value given above represents an upper bound. The corresponding LFL and stoichiometric laminar flame speeds for H_2 - C_6H_6 mixtures calculated using eqn. (4) are 0.62 and 2.8 ft/s (60/40 mixture) and 0.48 and 2.2 ft/s (40/60 mixture). Linear interpolation was used for intermediate compositions, which gives:

$$R_{v,l} (60\% H_2 - 40\% C_6H_6) = -1.23 + 67.4 \cdot (y_{c,l}) \quad (6)$$

and,

$$R_{v,l} (40\% H_2 - 60\% C_6H_6) = -1.41 + 84.3 \cdot (y_{c,l}) \quad (7)$$

where: $y_{c,l}$ = Total combustible mole fraction ($H_2 + C_6H_6$)

The laminar flame speeds given in Table 1 were calculated using these expressions. Note that no reduction in the laminar flame speed for Case 19a was taken to account for the inerting effect of water vapor; as shown in Figure 5, this is slightly conservative.

2.2.2 Best-Estimate Compositions

The best-estimate gas mixtures have significant levels of inert components (N_2 and H_2O); most of these mixtures are more heavily inerted than those shown in Figures 5 and 6. In addition, for the cases where the combustible concentrations exceeds the LFL, the mixtures are all significantly hyperstoichiometric. The upper bound H_2 and C_6H_6 laminar flame speeds based on the data shown in Figures 5 and 6 were taken to be 100 and 20 cm/s, respectively (3.3 and 0.66 ft/s), which gives a mixture laminar flame speed of 1.1 ft/s for a 50/50 mixture [eqn. (4)]; this value was employed for all the best-estimate gas composition calculations.

2.3 Turbulent Flame Speed Multiplier

The benchmark calculations discussed in Thomas (1993) for the hydrogen dewar deflagration experiments gave a turbulent flame speed multiplier of approximately 2. Since the hydrogen dewar has approximately the same gas volume as a half-filled waste tank and the tests were conducted with a number of internal structures (instrument platform, catwalks, ladders, etc.), it is reasonable to expect that the multiplier for a waste tank deflagration would be similar. The small adiabatic spherical container benchmark calculations discussed in Thomas (1993) demonstrate that internal structures are required to induce sufficient turbulence in the reactant gas to significantly accelerate the flame front.

It is recognized that the turbulent flame speed multipliers much greater than 2 have been reported in the literature. However, many of these values are for experiments conducted with open containers (Moen et al. 1981) and, as discussed in Thomas (1993), these are not relevant to a waste tank deflagration. Experiments with large fractions of the flow area blocked off also will not provide data applicable to this analysis. The volume represented by the cooling coils is less than 0.4% of the total internal volume enclosed by the primary liner. If the coils were configured in a triangular array, then the tube pitch would be approximately 4.5' and the flow area reduction at the midplane of a tube row would be 4.4%.

Based on these considerations, a turbulent flame speed multiplier of 2.5 is judged to be slightly conservative for a waste tank deflagration and was employed in this evaluation for both the air mixtures and best estimate gas compositions.

2.4 Autoignition Temperature

DPAC treats autoignition as an instantaneous event; once the reactant gas temperature reaches the AIT, all remaining reactant gas is assumed to combust instantaneously (Hensel 1993). In reality, this combustion requires some finite amount of time and the treatment employed by DPAC is thus conservative. The reactant gas temperature would have to significantly exceed the AIT values employed in this analysis in order for the reaction time to decrease to the point where the instantaneous event treatment would be realistic.

The AIT for a particular combustible gas is not a constant, but varies with pressure and composition. The AIT for H₂-air mixtures increases with the addition of H₂O or N₂, shows only a weak dependence of H₂ concentration for hypostoichiometric mixtures, increases sharply for with H₂ concentration for highly hyperstoichiometric mixtures, and decreases slightly with increasing pressure beyond 1 atmosphere (Jost 1946). Coward (1950) reports data showing that H₂-air mixtures at atmospheric pressure autoignite at 630°C with a lag time of 1/2 sec., at 585°C with a lag time of 5 sec., and at 572°C with a lag time of 15 seconds; he denotes 585°C as the "ignition point" and 630°C as the "rapid ignition point." Considering the DPAC treatment and deflagration time scale, the 630°C value would be a lower bound for the AIT. Coward (1950) gives 710°C as the rapid ignition point for C₆H₆-air mixtures. Sherman (1984) gives an H₂-air mixture AIT of 600°C.

Based on the discussion and data given above, an AIT of 600°C is judged to be conservative was employed for all mixtures in this analysis.

2.5 Waste Tank Vent Area

Tanks 48 and 49 have total vent areas of 27.15 and 60.48 ft², respectively (Estochen 1993). Based on the mass on the vent plugs and ignoring inertial effects, all of this area would be opened at a gas pressure of 13 psig. Much of the area would actually become available at lower pressures; however, since the gas pressure increases to 13 psig very quickly and inertial effects were ignored, the vent area was set to zero for lower pressures.

2.6 Waste Tank Fill Levels

With respect to safety analysis of the waste tanks, a fill level of 1/2 is assumed to represent an average condition and hence is of particular interest in this evaluation. Fill levels of 1/10, 1/2 and 3/4 were evaluated for the air mixtures. The 1/10 value was selected as a lower bound based on the expected operating conditions for Tank 48 (Walker 1993). The 3/4 value was chosen to illustrate the reduction in pressure at high fill levels. For the best-estimate gas compositions, the fill levels examined correspond to those for which the gas compositions were calculated (e.g. 50% for Tank 49 and 10% for Tank 48).

2.7 Initial Conditions

An initial gas temperature of 40°C was assumed for all of the air mixtures and for the normal best-estimate gas compositions. The tank 48 best-estimate gas composition for the peak C₆H₆ evolution rate corresponds to a gas temperature of 60°C, and hence this value was also used as the initial temperature in the pressure calculations. An initial gas pressure of 1 atmosphere was assumed for all calculations.

2.8 Primary Liner Pressure-Volume Data

The primary liner pressure-volume data were taken from the waste tank finite element structural analyses (Gong and Pelfrey 1993). Two data sets were employed in this evaluation. All cases were initially analyzed using the pressure-volume data from the finite element model in which the concrete construction joints are assumed to be intact. For cases where the calculated peak pressure exceeded 19 psig, the pressure at which the joints are assumed to fail (Gong and Pelfrey 1993), a new pressure was calculated using the pressure-volume data from the finite element model in which the concrete construction joints are assumed to be completely disconnected. It should be noted that deformation of the primary liner has only a small effect on the pressures calculated in this evaluation. For example, at 25 psig, the primary liner volume increase is less than 4% (assuming the joints have completely failed); much higher pressures would be required for primary liner deformation to have a large effect.

2.9 Other DPAC Inputs

All DPAC runs discussed in this report were made with a constant time step size of 2 msec and a convergence control parameter of 1×10^{-5} . The gas and effective emittance correlations, gas specific heat correlations, standard-state enthalpy of reaction values, combustion chemistry relationships, and tank volume and surface area values employed in DPAC were taken from Thomas (1993).

3.0 RESULTS AND DISCUSSION

It is useful to discuss the DPAC venting and autoignition models prior to presenting the results. Venting is turned off when the pressure drops below either: 1) the pressure required to accelerate the flow through the vents above Mach 0.5, or 2) the pressure at which the vents initially open (13 psig). For the conditions of interest in this evaluation, the pressure to open the vents controls so that venting is shut off when the tank pressure drops below 13 psig (the pressure may drop slightly below this value since energy will still be dissipated via radiative heat transfer). The maximum gas pressure occurs at the end of the burn due to autoignition for most cases where the pressure is artificially prevented from dropping by shutting off venting. As a result of these factors, a change in an input parameter which would physically be expected to lower the peak gas pressure (e.g. decreased flame speed, decreased energy release, increased energy dissipation, etc.) may have no effect on the calculated pressure for cases where venting is shut off for a portion of the burn or may even result in a slight increase; the burn time, however, will increase as expected. Similarly, changes which would physically be expected to raise the peak gas pressure may have no significant effect. It should be noted that this anomaly could be removed by incorporating a frictional flow model into DPAC for lower gas pressures; however, this would only decrease the pressure for the cases where the gas pressure is already quite low (< 20 psig) and hence would have no practical impact of the conclusions of this evaluation with regards to the structural integrity of the ITP waste tanks.

3.1 Air Mixtures

3.1.1 Air Mixture Compositions - Base Case Results

DPAC calculations were performed for each of the cases listed in Table 1; the calculated peak pressures and burn times are given in Table 3. The highest calculated peak gas pressures are for the stoichiometric mixtures since these give the largest energy releases and highest flame speeds. The peak pressure for a stoichiometric air mixture at a 1/2 fill level is less than 17 psig for both tanks. The peak pressures are also less than 17 psig for tank 49 at the 1/10 and 3/4 fill levels and for tank 48 at a 3/4 fill level. The peak calculated pressures for mixtures near the LFL in tank 48 at a 1/10 fill level are similar to those for the other fill levels, but those for mixtures near the stoichiometric condition are slightly higher. A stoichiometric dry air mixture in tank 48 at a 1/10 fill level (Case 19) gives a peak calculated pressure of 23.0 psig, which is the largest pressure calculated for all of the base air mixture cases. The pressure calculated for Case 19 with the "intact

joint" pressure-volume data for the primary liner were above 19 psig (24.2 psig), so this case was rerun with the data from the "disconnected joint" model. Accounting for the water vapor content of the air (Case 19a) gives a peak calculated pressure of 21.3 psig; this value is recommended as an upper-bound on the gas pressure which would result from a deflagration.

For most of the air mixture analyses, venting is shut off for a portion of the burn time and the peak pressure occurs at the end of the burn due to autoignition. For Tank 48 with a 1/10 fill height, the energy release is large enough (due to the large gas volume) and the vent area is small enough that as the mixture composition approaches the stoichiometric condition, venting is active during the entire burn so that increasing the combustible gas concentration results in a non-negligible increase in peak gas pressure. This is illustrated in Figure 8 where the gas pressures are plotted against fractional burn time (time divided by the total burn time) for Cases 15 through 19. The pressure time histories for tank 48 with stoichiometric air mixtures at fill heights of 1/2 and 1/10 and for an LFL mixture air mixtures at fill height of 1/10 are given in Appendix B.

The burn times decrease as the combustible concentration increases from the LFL up to the stoichiometric value due to the increase in flame speed and energy release. The burn times for the Tank 48 are longer than those for Tank 49 because the H_2 / C_6H_6 ratio is lower, and hence the flame speed is slower, even though the vent area for Tank 48 is smaller. The burn times increase with fill height since, as discussed in Section 3.1.2, the fraction of energy dissipated via venting and radiative heat transfer increases with fill height.

3.1.2 Air Mixture Compositions - Parametric Results

To illustrate the sensitivity of the calculated pressures to the key input values, a set of parametric calculations was performed for a stoichiometric-air mixture in tank 48 at a 1/2 fill level and an initial gas temperature of 60°C. Tank 48 was selected for the parametric study since it has the smaller vent area and a stoichiometric mixture was employed since it gives the largest energy release and highest flame speed. Flame speed, vent area, AIT, effective emittance, fill level, and the H_2 / C_6H_6 ratio were all varied. The results are given in Table 4; both the parameter value and the ratio of the parameter value to the nominal value are given in the table. Figures 9 and 10 show the calculated peak pressures and burn times. The results for each parameter are discussed below. It should be noted that the parametric results discussed below are only strictly applicable to the nominal value set

with which they were generated (e.g. gas composition, vent area, fill level, AIT and initial gas temperature). In general, the pressures calculated with non-stoichiometric mixtures, partially inerted mixtures, larger vent areas, higher fill levels, or higher AIT values will be less sensitive to variations in input values than the case discussed here.

Flame Speed [R_v]: Decreasing the input flame speed below the nominal value does not decrease the peak gas pressure although the burn time increases significantly. Increasing the time required to complete combustion beyond the base case value does not decrease the resulting gas pressure because venting does not occur continuously in the base case and the peak pressure occurs at the end of the burn due to autoignition. This behavior is also evident with some of the other parameters discussed below. As discussed previously, this is an artificial construct of the model since venting is turned off when the pressure drops below the value required to initially open the vents. Increasing the input flame speed raises the calculated peak gas pressure (venting occurs over the entire burn time at the higher flame speeds). Increasing the nominal flame speed by 50% increases the calculated peak gas pressure by less than 2 psi for this case.

Vent Area [A_v]: Increasing the available vent area does not change either the calculated peak gas pressure or burn time since venting does not occur continuously in the base case. Decreasing the vent area results in continuous venting and increases the peak pressure since less gas escapes. The burn time also decreases as the vent area is decreased since the product gas expansion and hence the flame front velocity increase; the decrease in burn time also decreases the amount of energy dissipated radiatively and hence contributes to the increase in gas pressure. Decreasing the vent area by 50% only increases the calculated peak gas pressure by 5 psi, but further decreases in vent area have a stronger effect.

Autoignition Temperature [AIT]: Increasing the autoignition temperature decreases the calculated peak gas pressure and increases the burn time since the calculated peak gas pressure for the base case occurs at the end of the burn due to autoignition. Decreasing the AIT from the base case value of 600°C to 500°C increases the peak gas pressure by 3 psi. It should be noted that the actual dependence of peak gas pressure on AIT for this case would actually be less than shown here since, as discussed above, the gas pressure is artificially supported at a critical value by turning off venting.

Effective Emittance [ϵ_{eff}]: The gas and effective emittance correlations developed in Thomas (1993) are used by DPAC; for the purposes of the parametric study, an effective emittance multiplier was temporarily instituted in DPAC to allow the emittance value to be scaled from the base case. The burn time increases slightly with emittance since increased radiative heat transfer decreases the temperature of the product gas and hence decreases the component of the flame front velocity due to product gas expansion. However, the calculated gas pressures increase slightly with emittance, which is not consistent with physical expectations; this anomaly is an indirect result of the venting model. Decreasing emittance increases the gas pressure in the initial portions of the burn so that the vents are opened earlier and remain above the venting pressure threshold for a longer period of time; this results in a larger total mass flow through the vents and hence a lower gas pressure. Conversely, increasing emittance delays the opening of the vents and results in venting being shutoff for a longer portion of the burn. For example, the fraction of the total gas mass which is

vented during the burn decreases from 77% for a zero emittance (adiabatic case) to 64% for the nominal emittance values.

Waste Solution Fill Level [F]: The fraction of the total energy released which is dissipated by venting and radiation increases with the waste solution fill level. This occurs because the total energy release decreases linearly with fill level, while the available vent area is independent of fill level and the radiative heat rate decreases with fill level but not as quickly as the energy release (Thomas 1993). The burn time increases with fill level due to the decrease in the product gas expansion component of the flame front velocity. For this case, decreasing the fill level from 1/2 to 1/10 increases the calculated peak gas pressure by less than 4 psi.

Combustible Gas Hydrogen Fraction [$y_c(H_2)$]: The main effect of increasing the fraction of hydrogen in the combustible gas (e.g. increasing the H_2/C_6H_6 ratio) is to increase the mixture flame speed since the flame speed for a stoichiometric H_2 -air mixture is much larger than that for a C_6H_6 -air mixture (see Figs. 5 & 6); the influence of flame speed was discussed above. This effect is offset slightly since the AICC pressure resulting from combustion of a stoichiometric H_2 -air mixture is less than that for a stoichiometric C_6H_6 -air mixture due to differences in the volumetric energy release, product gas specific heat, and product to reactant mole ratio (Thomas 1993). It should also be noted that combustible gas concentration for a stoichiometric mixture increases with the H_2/C_6H_6 ratio so that it would require a longer period of time after loss of ventilation to obtain a stoichiometric H_2 -rich mixture.

3.2 Best-Estimate Mixtures

DPAC calculations were performed for each of the cases listed in Table 2. Calculations were performed with the nominal flame speed ($R_v = 2.75$ ft/s from Sections 2.2 and 2.3), and with 2 times the nominal value (5.50 ft/s) in order to illustrate the effect of increased flame speed. The calculated peak pressures and burn times are given in Table 5 and are discussed below. The AICC pressures, calculated using the method discussed in Thomas (1993), are also shown in Table 2.

3.2.1 Best-Estimate Mixtures - Best-Estimate Flame Speeds

The maximum pressure for the best-estimate mixtures calculated using the best-estimate flame speed is 15.1 psig. The gas pressures for Tank 49 decrease with time after loss of ventilation; this occurs because the mixture becomes very rich due to the high combustible gas generation rate. For Tank 48 in the peak C_6H_6 generation rate condition, the first pressure given in Table 5 (1 day) is below that required to open the vents (13 psig); the calculated pressure is close to the AICC value since no gas is lost by venting and the gas temperatures are low enough that radiative heat transfer is not significant (the AICC gas temperatures for this case is 440K). For all the other cases, the pressure rises sufficiently to open the vents, but venting is shut off for a portion of the burn since the gas pressure does not rise significantly above this value and the peak pressure occurs at the end of the

burn due to autoignition. The burn times for these cases are very long (16 to 30 seconds) and would be even longer if DPAC were modified to allow continuous venting.

3.2.2 *Best-Estimate Mixture - Increased Flame Speeds*

Increasing the input flame speed by a factor of 2 does not increase the calculated peak gas pressure. Increasing the flame speed decreases the burn time, but this has little impact on the most of the calculated peak gas pressures since venting was shut off during a portion of the burn for the nominal flame speed cases. The calculated maximum gas pressures actually decrease in a few cases since the vents open sooner and remain open a larger fraction of the burn time. These results demonstrate that the calculated peak gas pressures for the best-estimate calculations are relatively insensitive flame speed variations.

3.3 Conservatisms & Uncertainties

There are a number of conservative features in the DPAC code and the input values employed in this analysis which should be considered along with the results presented above. Similarly, some uncertainties exist in the models and input parameters which should be noted. These are discussed below along with a qualitative assessment of their impact on the results of this analysis; the conservatisms and uncertainties are listed in order of importance.

3.3.1 *Conservatisms*

Consideration of Air Mixtures: Consideration of air mixtures (Section 3.1) is very conservative since this approach completely neglects the large amount of N_2 present in the tank vapor space at the time the ventilation system is lost and the air H_2O content. The air mixtures represent an upper bound with respect to the gas pressure resulting from a deflagration and should be treated as such. It is therefore appropriate that best-estimate values be used as inputs for the air mixture cases.

Consideration of Non-Combustible Best-Estimate Mixtures: As noted in Section 3.2, the best-estimate gas mixtures were treated as combustible without regard to the LFL, MOC, or UFL. However, many of these mixtures are not flammable. For these cases, a very strong ignition source might partially combust the gas in the immediate vicinity of the source, but the flame would not propagate and the resulting gas pressure increase would be insignificant. Thus, calculating pressures for best-estimate mixtures which are below the LFL or MOC, or above the UFL, is an extremely conservative approach.

Calculation of Mixture Laminar Flame Speed Mixture: The mixture laminar flame speed was calculated from the component laminar flame speeds using eqn. (4). The experimental data discussed in Section 2.2 indicates that this is a conservative approach. If additional experimental data on the flame speeds of combustible gas mixtures was obtained, it is anticipated that a less conservative model could be developed. Decreasing the mixture laminar flame speed would tend to increase the

burn time and decrease the peak gas pressure. However, as shown in Sections 3.1.2 and 3.2.2, minor laminar flame speed variations would not have a significant impact of the calculated gas pressures

Assumed Complete Combustion: For all the analyses reported here, it was assumed that the mixture would completely combust (e.g. consume all of the fuel in hypostoichiometric mixtures and all of the oxygen in hyperstoichiometric mixtures). However, experimental data for H₂-air mixtures shows that combustion of very lean mixtures near the LFL results in a significant fraction of uncombusted fuel; the H₂ concentration must be approximately 10% before the combustion process can be characterized as 100% complete without introducing a significant conservatism (Sherman 1984, Ratzel 1985, Marshall 1986, and Carcassi et al. 1987). Similarly, the data reported by Ratzel (1985) shows that very rich mixtures do not completely combust. Adjusting the energy release to account for incomplete combustion would lower the peak calculated gas pressures. The energy release values employed in this analysis are therefore conservative for the air mixtures near the LFL and for the best-estimate mixtures at the higher combustible gas concentrations.

Employed Upper-Bound Laminar Flame Speeds for Inerted and Near-Limit Compositions: The laminar flame speeds employed for mixtures near the flammability limits and for the heavily inerted best-estimate mixtures are conservative with respect to the trends of the data shown in Figures 5 and 6. For example, a laminar flame speed of 50 cm/s was used for the LFL H₂-air mixture (Section 2.2.1), whereas the data in Figure 5 indicates a much lower value. These conservative values were used since the data in these figures was being extrapolated. It is anticipated the input flame speed values could be reduced if additional data on near-limit and heavily inerted mixtures were obtained.

Neglected Venting for Pressures Below Critical Value: As discussed earlier, DPAC shuts off venting if the pressure drops below either: 1) the pressure required to accelerate the flow through the vents above Mach 0.5, or 2) the pressure at which the vents initially open (13 psig). This approach artificially supports the gas pressure at 13 psig for many of the cases examined. This restriction could be removed by transitioning to a compressible frictional flow model below the critical pressure and accounting for vent plug inertial effects; however, this would only decrease the pressure for the cases where the gas pressure is already quite low.

Flame Front Geometric Description: The flame front geometric model employed in DPAC is discussed in Thomas (1993). The model assumes that: (1) a vertical sheet of flame aligned radially and extending from the top of the tank to the waste solution surface would be established instantaneously at the beginning of the deflagration, (2) two flame fronts would propagate away from this vertical plane, and (3) the flame fronts would remain vertical and aligned radially as they propagated. This approach overestimates the flame front area, and hence the combustion rate and gas pressure, at the beginning of the burn and may slightly underestimate the flame front area in later stages of the burn. While this model is judged to be a reasonable description of the flame front geometry, accounting for the curvature of the flame front as it propagates away from the ignition point would give a smaller average flame front area and hence would increase the burn time and decrease the peak gas pressure.

Neglected Combustion Product Disassociation & Equilibrium Concentrations: As noted above, it was assumed in this analysis that the mixture would completely combust. Furthermore, it was assumed that none of the combustion products would dissociate

(e.g. the equilibrium reactant gas concentrations were ignored). Accounting for these factors would reduce the peak gas pressures.

Assumed Preferential Combustion of Hydrogen in Hyperstoichiometric Mixtures: For hyperstoichiometric mixtures of H_2 and C_6H_6 (e.g. all of the best-estimate compositions above the LFL), the combustion model assumes that all H_2 in a unit volume is reacted prior to any C_6H_6 combustion (Thomas 1993). This is conservative since H_2 combustion liberates more energy than C_6H_6 on a per mole of oxygen basis, as shown in Appendix A. However, the flame speeds for H_2 - C_3H_8 mixtures (Fig. 7), which have per mole of oxygen energy release values that are essentially the same as those for the H_2 - C_6H_6 system, indicate that H_2 is not preferentially combusted. Therefore, the energy releases for hyperstoichiometric mixtures employed in this evaluation are upper-bound values.

Neglected Energy Dissipated via Structural Deformation & Displacement: The energy required to deform the tank (particularly the liners) and displace the concrete top slab and center column was not accounted for in this analysis. This would not have a significant impact on the calculated pressures for the cases of interest in this evaluation; the results of a simplified bounding calculation indicate that less than 5% of the energy released from a stoichiometric H_2 -air mixture at $25^\circ C$ in a half-filled tank would be dissipated by this mechanism.

Use of Isothermal Product Gas Volume & Low Water Vapor Emittance Data: Several aspects of the radiative heat transfer model and data are conservative. The water vapor emittance data employed in this analysis are conservative in the high temperature regime ($> 2000K$), as discussed in Thomas (1993). The hot product gas region was treated as isothermal, with an average temperature assigned to the entire volume; this approach will slightly underpredict the radiative heat rate since it is proportional to the gas temperature raised to the fourth power.

Neglected Convection: Convection from the hot product gas to available surfaces was neglected in this analysis. It is anticipated that this heat transfer mode would be small compared to the radiative heat transfer during the deflagration so that this assumption is not a significant conservatism.

3.3.2 *Uncertainties*

Turbulent Flame Speed Multiplier: A turbulent flame speed multiplier of 2.5 was used as the best-estimate value in this evaluation. As discussed in Section 2.3, this value is judged to be slightly conservative with respect to the benchmark calculations described in Thomas (1993). It is recognized that there is some uncertainty in this value. However, increasing the flame speed by a factor of 2 has no effect on the peak gas pressure for the best-estimate mixtures.

Combined Effect of Temperature and Pressure on Flame Speed: As discussed in Section 2.2, it was assumed that the laminar flame speed was independent of temperature and pressure. This assumption was made on the basis that the reactant gas pressure and temperature both increase during the burn and the effects of temperature and pressure on flame speed offset one another. It is not anticipated that a more rigorous treatment would significantly change the flame speed values and, as shown by the sensitivity analyses discussed above, minor variations in flame speed will not have a large impact on the calculated pressures.

3.4 Comparison with Other Waste Tank Deflagration Pressure Evaluations

Wallace and Yau (1986) and Walker (1990) have calculated the gas pressure which would result from a waste tank deflagration assuming that the tank is an unvented adiabatic structure; in addition, Walker treated the tank as a rigid structure (e.g. an AICC treatment). In both cases air mixtures were assumed; Wallace and Yau considered a hypostoichiometric H_2 -air mixture while Walker evaluated stoichiometric mixtures of H_2 and C_6H_6 with air. The peak gas pressures calculated with these assumptions range from 62 (hypostoichiometric H_2 -air mixture) to 131 psig (stoichiometric C_6H_6 -air mixture). Since significant amounts of energy are dissipated via venting and radiation, these analyses give much higher gas pressures for air mixtures than reported here.

Prior to this work, a deflagration pressure analysis conducted by Westinghouse Nuclear and Advanced Technology Division (NATD) using the COMPACT code (Srinivas 1991) was considered for use in the ITP waste tank deflagration structural integrity evaluation. The work reported here was initiated because preliminary analyses indicated that radiative heat transfer, which was not accounted for in the NATD analyses, could significantly reduce the gas pressure resulting from a deflagration. As work on this task proceeded, it was also determined that the single gas volume approach implemented with COMPACT was not capable of accurately predicting burn time; to account for this, NATD employed a very high laminar flame speed so as to bound burn time. Furthermore, the single volume approach cannot model reactant gas heating due to compression and therefore cannot account for autoignition effects. As discussed in Appendix C, the effect of venting will be underpredicted with the single volume approach since the mass flow rate through the vents is inversely proportional the square root of the gas temperature. As a result of these effects, the gas pressures calculated by NATD are higher than those reported here.

The MELCOR/SR code was also employed as part of the effort to evaluate the gas pressure resulting from a deflagration in an ITP waste tank (Allison and Chow 1993). The MELCOR/SR model employed represented the gas volume as a single region, like the COMPACT code discussed above, and hence cannot accurately calculate burn times or vent rates. Unlike COMPACT, MELCOR/SR has the capacity to calculate radiative heat transfer from the gas. However, a single region model will underpredict the radiative heat transfer rate since it treats the gas as isothermal, as discussed in Appendix C. At equal burn times, the results obtained with COMPACT are comparable to those reported here (Allison and Chow 1993).

The preliminary results generated as part of this work (Thomas and Hensel 1993b, Hensel and Thomas 1993) gave larger peak gas pressures than those reported here. This is primarily due to the fact that very conservative laminar flame speeds were employed in this preliminary analyses since much of the literature flame speed data discussed in Section 2.2 was not available at the time the preliminary calculations were made. In addition, a conservative set of gas emittances were employed in the preliminary analyses since the gas emittance correlations taken from Thomas (1993) were not available.

4.0 CONCLUSIONS

The DPAC computer code was employed to calculate the pressure which would result from a deflagration in an ITP waste tank. Conservative flame speed, autoignition temperature, and emittance values were employed as input in this analysis. Mixtures of $H_2-C_6H_6$ with air were evaluated to establish an upper bound for the deflagration pressure. A parametric study was performed for a stoichiometric air mixture in Tank 48 at a 1/2 fill level in order to demonstrate the sensitivity of the calculated pressures to variations in the input data. Best-estimate calculations of the peak deflagration pressure were generated using gas composition data which account for the initial N_2 inerting, the water vapor content of the air, and oxygen intake due to atmospheric exchange mechanisms. The results reported here were compared with the results of previous analyses.

The calculated pressures for the air mixtures are less than 17 psig for both Tank 48 and 49 at a fill level of 1/2. Considering the effects of water vapor, the maximum calculated pressure for the air mixtures is 21 psig and occurs with a stoichiometric air mixture in Tank 48 at a fill level of 1/10. The maximum gas pressure calculated for the best-estimate gas mixtures with the best-estimate flame speed is 15.1 psig.

The parametric results demonstrate that the calculated peak pressures are not strongly sensitive to variations in the input parameters (e.g. flame speed, composition, vent area, autoignition temperature, gas emittance). Furthermore, the input parameters were selected in a conservative fashion to account for uncertainty in the experimental data. The venting, radiation, combustion, and flame front propagation models employed by DPAC also incorporate a number of implicit conservatisms. As a result, the calculated peak gas pressures are upper-bound values for a given mixture composition. The uncertainty in the pressures is therefore one-sided, and the pressures calculated with true best-estimate input data and models would be lower than those reported here.

Previous analyses of waste tank deflagration pressures have either neglected significant modes of energy dissipation (venting and radiation) and/or have treated the gas as a single region and therefore underpredicted the energy dissipation rates. Additionally, none of the previous analysis were capable of accurately calculating the burn time, so that the total energy dissipated via venting and radiation could not be accurately calculated. The analysis reported here provides a much more accurate evaluation of these energy dissipation modes and, as a result, gives significantly lower peak gas pressures.

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Table 1 Input Data for Upper-Bound Air Mixture Cases.

Case No.	Tank No.	Concentrations (%)					Flame Speeds (ft/s) [R _v]			Vent Area (ft ²)	Fill Level
		comb.	H ₂	C ₆ H ₆	O ₂	N ₂	Laminar	Turb. Mult.	Net		
1	49	2.76	1.66	1.10	20.42	76.82	0.63	2.5	1.6	60.48	1/2
2	49	3.57	2.14	1.43	20.25	76.18	1.18	2.5	2.9	60.48	1/2
3	49	4.37	2.62	1.75	20.08	75.55	1.72	2.5	4.3	60.48	1/2
4	49	5.18	3.11	2.07	19.91	74.91	2.26	2.5	5.7	60.48	1/2
5	49	5.98	3.59	2.39	19.74	74.28	2.80	2.5	7.0	60.48	1/2
6	49	2.76	1.66	1.10	20.42	76.82	0.63	2.5	1.6	60.48	1/10
7	49	5.98	3.59	2.39	19.74	74.28	2.80	2.5	7.0	60.48	1/10
8	49	2.76	1.66	1.10	20.42	76.82	0.63	2.5	1.6	60.48	3/4
9	49	5.98	3.59	2.39	19.74	74.28	2.80	2.5	7.0	60.48	3/4
10	48	2.24	0.90	1.34	20.53	77.23	0.48	2.5	1.2	27.15	1/2
11	48	2.75	1.10	1.65	20.42	76.83	0.91	2.5	2.3	27.15	1/2
12	48	3.26	1.30	1.96	20.32	76.42	1.34	2.5	3.3	27.15	1/2
13	48	3.77	1.51	2.26	20.21	76.02	1.77	2.5	4.4	27.15	1/2
14	48	4.28	1.71	2.57	20.10	75.62	2.20	2.5	5.5	27.15	1/2
15	48	2.24	0.90	1.34	20.53	77.23	0.48	2.5	1.2	27.15	1/10
16	48	2.75	1.10	1.65	20.42	76.83	0.91	2.5	2.3	27.15	1/10
17	48	3.26	1.30	1.96	20.32	76.42	1.34	2.5	3.3	27.15	1/10
18	48	3.77	1.51	2.26	20.21	76.02	1.77	2.5	4.4	27.15	1/10
19	48	4.28	1.71	2.57	20.10	75.62	2.20	2.5	5.5	27.15	1/10
19a	48	4.00	1.60	2.40	18.80	70.65	2.20	2.5	5.5	27.15	1/10
20	48	2.24	0.90	1.34	20.53	77.23	0.48	2.5	1.2	27.15	3/4
21	48	4.28	1.71	2.57	20.10	75.62	2.20	2.5	5.5	27.15	3/4

Note: [a] Case 19a assumes a stoichiometric mixture with a water vapor concentration equal to 90% of saturation $((0.9) \cdot (7.28\%) = 6.55\%)$.

Table 2 Gas Compositions Considering Initial Nitrogen and Water Vapor.

Case No.	Tank No.	Operating Condition	Time (days)	Reactant Gas Mole Fractions				combustibles (H ₂ + C ₆ H ₆)	Excess N ₂	Ratio O ₂ to Noncombustibles	LFL	Comb./LFL	Stoich.	Comb./Stoich.
				O ₂	N ₂	C ₆ H ₆	H ₂	H ₂ O						
1	49	Normal	3	0.0777	0.8255	0.0096	0.0144	0.0728	0.024	0.533	0.080	0.022	0.024	1.02
2	49	Normal	6	0.0902	0.7928	0.0177	0.0265	0.0728	0.044	0.453	0.094	0.022	0.027	1.62
3	49	Normal	12	0.1098	0.7413	0.0305	0.0456	0.0728	0.076	0.328	0.119	0.022	0.033	2.29
4	49	Normal	18	0.1240	0.7040	0.0397	0.0594	0.0728	0.099	0.238	0.138	0.022	0.038	2.64
5	49	Normal	24	0.1343	0.6771	0.0464	0.0694	0.0728	0.116	0.172	0.152	0.022	0.041	2.85
6	49	Normal	30	0.1417	0.6576	0.0512	0.0767	0.0728	0.128	0.125	0.162	0.022	0.043	2.98
7	48	Normal	3	0.0662	0.8564	0.0028	0.0018	0.0728	0.005	0.607	0.067	0.028	0.014	0.33
8	48	Normal	6	0.0693	0.8492	0.0053	0.0033	0.0728	0.009	0.589	0.070	0.028	0.014	0.60
9	48	Normal	12	0.0753	0.8355	0.0101	0.0064	0.0728	0.016	0.552	0.077	0.028	0.016	1.04
10	48	Normal	18	0.0808	0.8226	0.0145	0.0092	0.0728	0.024	0.519	0.083	0.028	0.017	1.41
11	48	Normal	24	0.0861	0.8105	0.0187	0.0119	0.0728	0.031	0.487	0.089	0.028	0.018	1.70
12	48	Normal	30	0.0910	0.7991	0.0227	0.0144	0.0728	0.037	0.457	0.095	0.028	0.019	1.95
13	48	Peak	1	0.0630	0.7425	0.0007	0.0001	0.1937	0.001	0.505	0.063	0.034	0.010	0.09
14	48	Peak	4	0.0626	0.7404	0.0033	0.0001	0.1937	0.003	0.505	0.063	0.037	0.009	0.39
15	48	Peak	4.25	0.0628	0.7367	0.0065	0.0003	0.1937	0.007	0.501	0.063	0.037	0.009	0.78
16	48	Peak	11.88	0.0760	0.7136	0.0122	0.0046	0.1937	0.017	0.428	0.077	0.031	0.014	1.23
17	48	Peak	18.13	0.0854	0.6971	0.0162	0.0076	0.1937	0.024	0.376	0.088	0.030	0.016	1.46
18	48	Peak	23.96	0.0932	0.6836	0.0195	0.0101	0.1937	0.030	0.333	0.096	0.029	0.018	1.62
19	48	Peak	29.79	0.1000	0.6716	0.0224	0.0123	0.1937	0.035	0.295	0.104	0.029	0.020	1.74

Table 3 Results for Upper-Bound Air Mixture Cases.

Case No.	Tank No.	Fill Level	Comb. Conc. [H ₂ + C ₆ H ₆] (%)	Conc. Note	Flame Speed (ft/s)	Peak Pressure (psig)	Burn Time (sec)
1	49	1/2	2.76	LFL	1.6	15.6	28.9
2	49	1/2	3.57	1/4	2.9	16.0	14.9
3	49	1/2	4.37	1/2	4.3	16.3	9.47
4	49	1/2	5.18	3/4	5.7	16.6	6.82
5	49	1/2	5.98	Stoich	7.0	16.8	5.35
6	49	1/10	2.76	LFL	1.6	15.6	28.6
7	49	1/10	5.98	Stoich	7.0	16.8	5.25
8	49	3/4	2.76	LFL	1.6	15.6	29.4
9	49	3/4	5.98	Stoich	7.0	16.7	5.53
10	48	1/2	2.24	LFL	1.2	15.9	38.6
11	48	1/2	2.75	1/4	2.3	16.2	18.6
12	48	1/2	3.26	1/2	3.3	16.5	12.3
13	48	1/2	3.77	3/4	4.4	16.7	8.82
14	48	1/2	4.28	Stoich	5.5	16.9	6.80
15	48	1/10	2.24	LFL	1.2	15.9	38.1
16	48	1/10	2.75	1/4	2.3	16.2	18.3
17	48	1/10	3.26	1/2	3.3	16.5	12.1
18	48	1/10	3.77	3/4	4.4	17.3	8.63
19	48	1/10	4.28	Stoich	5.5	23.0 [d]	6.50
19a	48	1/10	4.00 [e]	Stoich	5.5	21.3 [d]	6.70
20	48	3/4	2.24	LFL	1.2	15.9	39.3
21	48	3/4	4.28	Stoich	5.5	16.9	6.95

- Notes: [a] Initial conditions of 40°C and 1 atmosphere assumed for all cases.
 [b] Autoignition temperature set to 600°C for all cases.
 [c] Gas compositions and vent areas given in Table 1.
 [d] Calculated using primary liner pressure-volume data from the disconnected joint finite element structural model. The pressure and burn time calculated using the intact joint model data were 24.2 psig and 6.36 sec, respectively, for case 19, and 22.4 psig and 6.57 sec, respectively, for case 19a.
 [e] Case 19a assumes a stoichiometric mixture with a water vapor concentration equal to 90% of saturation $((0.9) \cdot (7.28\%) = 6.55\%)$.

Table 4 Parametric Analyses for Stoichiometric Air Mixture in Tank 48.

Parameter (see note [a])	Value	Fraction of Nominal	Peak Pressure (psig)	Burn Time (sec)
Flame Speed (ft/s) [R_v]	2.75	0.50	17.8	14.5
	4.125	0.75	17.7	9.31
	5.50	1.00	17.6	6.82
	8.25	1.50	18.9	4.34
	11.0	2.00	29.0	3.03
Vent Area (ft ²) [A_v]	6.788	0.25	46.7	6.11
	13.58	0.50	22.6	6.51
	20.36	0.75	17.6	6.80
	27.15	1.00	17.6	6.82
	33.94	1.25	17.6	6.82
	54.30	2.00	17.6	6.82
Autoignition Temp. (°C)	500	0.83	20.7	6.39
	600	1.00	17.6	6.82
	700	1.12	15.8	7.09
	800	1.33	14.8	7.27
	∞	∞	13.4	7.70
Effective Emittance [ϵ_{eff}]	[b]	0.00	17.3	5.97
	[b]	0.50	17.5	6.49
	[b]	0.75	17.5	6.67
	[b]	1.00	17.6	6.82
	[b]	1.25	17.6	6.94
	[b]	1.50	17.7	7.05
Waste Solution Fill Level [F]	0.10	0.20	21.5	6.49
	0.25	0.50	17.8	6.68
	0.50	1.00	17.6	6.82
	0.75	1.50	17.6	6.97
Combustible Gas Hydrogen Frac. [$y_c(H_2)$] (see note [c])	0.0	0.00	17.6	10.3
	0.4	1.00	17.6	6.82
	0.6	1.50	17.6	5.28
	0.8	2.00	20.3	3.77
	1.0	2.50	39.3	2.26

- Notes: [a] The input composition, fill level, and vent area for the base case are given in Table 1 (case 14). The initial temperature and pressure were 60°C and 1 atmosphere.
- [b] The effective emittance correlation in the code was multiplied by the given value (as opposed to setting the effective emittance to a fixed value).
- [c] Flame speed varies with gas composition. The values employed for these cases were 3.75, 5.5, 7.0, 9.5, and 15.5 ft/s.

Table 5 Results for Best Estimate Gas Compositions.

Case No.	Tank No.& Condition	Time (days)	Peak Gas Pressure (psig)			Burn Time (sec)	
			R _v = 2.75 ft/s	R _v = 5.50 ft/s	AICC	R _v = 2.75 ft/s	R _v = 5.50 ft/s
1	49-Normal	3	15.1	15.0	60.6	17.1	8.27
2	49-Normal	6	15.0	15.0	65.3	16.8	8.08
3	49-Normal	12	14.9	14.9	71.3	16.3	7.85
4	49-Normal	18	14.8	14.7	74.9	16.1	7.72
5	49-Normal	24	14.5	14.5	77.1	16.2	7.77
6	49-Normal	30	14.5	14.5	78.6	16.2	7.74
7	48-Normal	3	13.7	13.7	19.2	22.9	11.4
8	48-Normal	6	14.2	14.2	34.8	19.5	9.60
9	48-Normal	12	15.0	15.0	58.7	17.0	8.28
10	48-Normal	18	14.9	14.9	60.5	16.9	8.18
11	48-Normal	24	14.9	14.9	62.1	16.7	8.09
12	48-Normal	30	14.9	14.8	63.5	16.6	8.02
13	48-Peak	1	3.73	3.82	4.64	29.6	14.8
14	48-Peak	4	13.8	13.8	19.5	23.0	11.4
15	48-Peak	4.25	14.4	14.4	36.6	19.4	9.55
16	48-Peak	11.9	14.9	14.9	52.7	17.6	8.58
17	48-Peak	18.1	15.0	15.0	56.9	17.3	8.38
18	48-Peak	24.0	15.0	15.0	60.2	17.0	8.24
19	48-Peak	29.8	15.0	15.0	62.9	16.8	8.13

- Notes: [a] Gas mixture compositions given in Table 2.
 [b] Initial gas temperature of 40°C for Cases 1 - 12, and 60°C for Cases 13 - 19.
 Initial gas pressure of 1 atmosphere for all cases.
 [c] Vent area of 60.48 square ft. for Tank 49 and 27.15 square ft. for Tank 48.
 [d] Waste solution fill heights of 0.5 for Tank 49 and 0.1 for Tank 48.
 [e] AIT value of 600°C for all cases.

Figure i Type IIIA Waste Tank Cross Section (SRS 1991).

Figure 2 Tank 49 Gas Composition - Normal Condition.

Figure 3 Tank 48 Gas Composition - Normal Condition.

Figure 4 Tank 48 Gas Composition - Peak C₆H₆ Gen. Rate Condition.

Figure 5 Hydrogen-air mixtures flame speeds (Lewis and Von Elbe 1961).

Figure 6 Benzene-air mixtures flame speeds (Golovina and Fyodorov 1957).

Figure 7 Propane-hydrogen-air mixtures flame speeds (Leason 1953).

Figure 8 Gas Pressure Histories: Tank 48, dry air mixtures, 1/10 full.

Figure 9 Parametric Gas Pressure Results (Tank 48, stoich. H2-air mixture, 1/2 full, 60°C).

Figure 10 Parametric Burn Time Results (Tank 48, stoich. H2-air mixture, 1/2 full, 60°C).

Appendix A - Standard-State Enthalpy of Reaction Values

This appendix presents the calculation of the standard-state enthalpy of reactions values for combustion of hydrogen, benzene, and propane-air mixtures. Ignoring non-oxygen air components and secondary reactions among products and reactants, the combustion reactions may be written as:

The standard-state enthalpy of reaction can be computed from the standard-state enthalpies of formation for the products and reactants, as shown below:

$$\Delta h_r^\circ = \left(\sum N_j \Delta h_{f,j}^\circ \right)_{\text{products}} - \left(\sum N_j \Delta h_{f,j}^\circ \right)_{\text{reactants}} \quad (\text{A4})$$

where: Δh_r° = Standard-state enthalpy of reaction,
 N_j = Number of moles of jth species, and
 $\Delta h_{f,j}^\circ$ = Standard-state enthalpy of formation of jth species.

Wark (1977) gives the standard-state (25°C, 1 atm.) enthalpies of formation for CO₂, H₂O, C₆H₆, and C₃H₈ as -393,520, -241,820, +82,930, and -103,850 kJ/kg-mole, respectively. The standard-state enthalpy of reaction values calculated using these values with eqn. (A4) are given below in Table A1. As shown in the table, the values for propane and benzene are similar on a per mole of oxygen basis, while that for hydrogen is significantly larger.

Table A1 Standard-State Enthalpy of Reaction Values.

Fuel	Standard-State Enthalpy of Reaction (kcal/g-mole)	
	per mole of fuel	per mole of oxygen
H ₂	57.80	115.6
C ₆ H ₆	757.5	101.0
C ₃ H ₈	488.5	97.7

Appendix B - Time Histories for Selected Cases

This appendix presents the time histories of the calculated gas pressures, volumes, temperatures, emittances, radiative heat fluxes, radiative heat rates, and venting rates for dry air mixtures in Tank 48 at fill level - combustible gas concentrations of: 1/2 - stoichiometric (Case 14, Figures B1 through B4), 1/10 - LFL (Case 15, Figures B5 through B8), and 1/10 - stoichiometric (Case 19, Figures B9 through B12). These cases are discussed in Section 3.1.1 of this report.

The data used to construct these plots corresponds to 0.2 second time intervals so that some of the curves are not completely smooth. The effect of turning venting on and off as the gas pressure drops below the value required to initially open the vents (13 psig) is evident in the mass flow rates through the vents for Cases 14 and 15 (Figs. B3 & B7); venting is continuous for Case 19 (Figure B11).

Figure B1 Case 14 Upper-Bound Air Mixture, Gas Pressure and Temperatures.

Figure B2 Case 14 Upper-Bound Air Mixture, Product & Reactant Masses and Volumes.

Figure B3 Case 14 Upper-Bound Air Mixture, Vent Rates and Radiative Heat Rate.

Figure B4 Case 14 Upper-Bound Air Mixture, Gas Emittances and Radiative Heat Fluxes.

Figure B5 Case 15 Upper-Bound Air Mixture, Gas Pressure and Temperatures.

Figure B6 Case 15 Upper-Bound Air Mixture, Product & Reactant Masses and Volumes.

Figure B7 Case 15 Upper-Bound Air Mixture, Vent Rates and Radiative Heat Rate.

Figure B8 Case 15 Upper-Bound Air Mixture, Gas Emittances and Radiative Heat Fluxes.

Figure B9 Case 19 Upper-Bound Air Mixture, Gas Pressure and Temperatures.

Figure B10 Case 19 Upper-Bound Air Mixture, Product & Reactant Masses and Volumes.

Figure B11 Case 19 Upper-Bound Air Mixture, Vent Rates and Radiative Heat Rate.

Figure B12 Case 19 Upper-Bound Air Mix, Gas Emittances and Radiative Heat Fluxes.

Appendix C - Single vs. Two Region Venting & Radiative Heat Transfer

This appendix presents a comparison of the venting and radiative heat transfer rates calculated with the waste tank gas volume modeled as a single region (product and reactant gases perfectly mixed) vs. those calculated with a two-region model (product and reactant gases treated as separate control volumes). The code developed in this work (DPAC) uses a two-region model, whereas the deflagration analyses which employed the MELCOR/SR (Allison and Chow 1993) and COMPACT (Srinivas 1991) codes utilized single region models. It is emphasized that the two-region model is physically more representative of a waste tank deflagration, and that this comparison is made only to understand the magnitude of the differences in the venting and radiative heat transfer rates calculated with the two models.

The most important difference between the single- and two-region approaches is that it is not possible to calculate burn time with a single-region model from experimental flame speed data; the single-region approach cannot model the expansion of the product gas, which dominates the flame front velocity (Thomas 1993). However, it is possible to compare the results of the single- and two-region models on an equal burn time basis (e.g. the burn time from the two-region model is used to define the input flame speed for the single-region model); this was the approach used by Allison and Chow (1993) to compare the results from DPAC and MELCOR/SR.

To a first approximation the mass flow rates through the vents, assuming isentropic flow, is proportional to the inverse of the square root of the gas temperature (Hensel 1993). Similarly, neglecting the temperature dependence of the emittance coefficients, the radiative heat transfer rate is proportional to the fourth power of the gas temperature. If the waste tank vapor space is modeled as a single perfectly mixed gas region, then the venting and radiative heat transfer rates can be written as:

$$\dot{m}_1 = \frac{A}{\sqrt{T_a}} \quad (C1)$$

$$Q_1 = B T_a^4 \quad (C2)$$

where: $\dot{m}$ = Mass flow rate through the vents,
A = Proportionality constant for venting,
 T_a = Average gas temperature,
Q = Radiative heat transfer rate, and
B = Proportionality constant for radiative heat transfer.

The '1' subscript denotes the single-region model. The average gas temperature, defined on a volumetric (molar) basis, can be expressed as:

$$T_a = V_{f,r} T_r + V_{f,p} T_p \quad (C3)$$

where: $V_{f,r}$ = Reactant gas volume fraction ($0 \leq V_{f,r} \leq 1$),
 T_r = Reactant gas temperature,
 $V_{f,p}$ = Product gas volume fraction ($0 \leq V_{f,p} \leq 1$, $V_{f,p} + V_{f,r} = 1$),
 T_p = Product gas temperature.

Substituting this expression into the single-region rate equations (C1 and C2) gives:

$$\dot{m}_1 = \frac{A}{\sqrt{V_{f,r} T_r + V_{f,p} T_p}} \quad (C4)$$

$$Q_1 = B (V_{f,r} T_r + V_{f,p} T_p)^4 \quad (C5)$$

Assuming that the vent area and radiative heat sink surfaces are uniformly distributed, the two-region venting and radiative heat transfer rates can be written as:

$$\dot{m}_2 = A \left(\frac{V_{f,r}}{\sqrt{T_r}} + \frac{V_{f,p}}{\sqrt{T_p}} \right) \quad (C6)$$

$$Q_2 = B (V_{f,r} T_r^4 + V_{f,p} T_p^4) \approx B (V_{f,p} T_p^4) \quad (C7)$$

If the flame front velocity is constant over the course of the burn, then the reactant and product gas volume fractions are linear with burn time, as shown below:

$$V_{f,r} = 1 - t / t_b \quad (C8)$$

$$V_{f,p} = t / t_b \quad (C9)$$

where: t = Time, and
 t_b = Burn time (total time required to complete the deflagration).

The single- and two-region rate equations (C4 - C7) can then be written as:

$$\dot{m}_1(t) = \frac{A}{\sqrt{T_r + \frac{1}{t_b} (T_p - T_r)}} \quad (C10)$$

$$Q_1(t) = B \left(T_r + \frac{1}{t_b} (T_p - T_r) \right)^4 \quad (C11)$$

$$\dot{m}_2(t) = A \left[\frac{1}{\sqrt{T_r}} + \frac{1}{t_b} \left(\frac{1}{\sqrt{T_p}} - \frac{1}{\sqrt{T_r}} \right) \right] \quad (C12)$$

$$Q_2(t) = B \left(\frac{1}{t_b} T_p^4 \right) \quad (C13)$$

The average rates can then be found as shown below:

$$\begin{aligned} \bar{m}_1 &= \frac{1}{t_b} \int_0^{t_b} \dot{m}_1(t) dt = \frac{A}{t_b} \int_0^{t_b} \left[T_r + \frac{1}{t_b} (T_p - T_r) \right]^{-1/2} dt \\ \bar{m}_1 &= \frac{A}{t_b} \left(\frac{2 t_b}{(T_p - T_r)} \sqrt{T_r + \frac{1}{t_b} (T_p - T_r)} \right) \Big|_0^{t_b} = 2 A \left(\frac{\sqrt{T_p} - \sqrt{T_r}}{T_p - T_r} \right) \end{aligned} \quad (C14)$$

$$\begin{aligned} \bar{Q}_1 &= \frac{1}{t_b} \int_0^{t_b} Q_1(t) dt = \frac{B}{t_b} \int_0^{t_b} \left(T_r + \frac{1}{t_b} (T_p - T_r) \right)^4 dt \\ \bar{Q}_1 &= \frac{B}{t_b} \left(\frac{t_b}{5(T_p - T_r)} \left(T_r + \frac{1}{t_b} (T_p - T_r) \right)^5 \right) \Big|_0^{t_b} = \frac{B}{5} \left(\frac{T_p^5 - T_r^5}{T_p - T_r} \right) \approx \frac{B}{5} \left(\frac{T_p^5}{T_p - T_r} \right) \end{aligned} \quad (C15)$$

$$\begin{aligned} \bar{m}_2 &= \frac{1}{t_b} \int_0^{t_b} \dot{m}_2(t) dt = \frac{A}{t_b} \int_0^{t_b} \left[\frac{1}{\sqrt{T_r}} + \frac{1}{t_b} \left(\frac{1}{\sqrt{T_p}} - \frac{1}{\sqrt{T_r}} \right) \right] dt \\ \bar{m}_2 &= \frac{A}{t_b} \left(\frac{1}{\sqrt{T_r}} + \frac{t^2}{2 t_b} \left(\frac{1}{\sqrt{T_p}} - \frac{1}{\sqrt{T_r}} \right) \right) \Big|_0^{t_b} = \frac{A}{2} \left(\frac{1}{\sqrt{T_r}} + \frac{1}{\sqrt{T_p}} \right) = \frac{A}{2} \left(\frac{\sqrt{T_p} + \sqrt{T_r}}{\sqrt{T_p T_r}} \right) \end{aligned} \quad (C16)$$

$$\bar{Q}_2 = \frac{1}{t_b} \int_0^{t_b} Q_2(t) dt = \frac{B}{t_b} \int_0^{t_b} \left(\frac{1}{t_b} T_p^4 \right) dt = \frac{B}{2} T_p^4 \quad (C17)$$

The ratios of the two-region to single-region venting and radiative heat transfer rates may therefore be expressed using eqns. (C14) through (C17) as:

$$\frac{\bar{m}_2}{\bar{m}_1} = \frac{\frac{A}{2} \left(\frac{\sqrt{T_p} + \sqrt{T_r}}{\sqrt{T_p T_r}} \right)}{2 A \left(\frac{\sqrt{T_p} - \sqrt{T_r}}{T_p - T_r} \right)} = \frac{(T_p - T_r)(\sqrt{T_p} + \sqrt{T_r})}{4 \sqrt{T_p T_r} (\sqrt{T_p} - \sqrt{T_r})} \quad (C18)$$

$$\frac{\bar{Q}_2}{\bar{Q}_1} = \frac{\frac{B}{2} T_p^4}{\frac{B}{5} \left(\frac{T_p^5}{T_p - T_r} \right)} = \frac{5}{2} \left(1 - \frac{T_r}{T_p} \right) \quad (C19)$$

Table C1 gives the mass flow rates through the vents and radiative heat transfer rates for the single- and two-region models as a function of the product and reactant gas volume fractions calculated using eqns. (C14) through (C17) for a product gas temperature of 3000 K and a reactant gas temperature of 300 K. The constant of proportionality was taken to be unity, so that the values shown in the table are normalized.

The mass flow rate through the vents decreases for both models as the product gas volume fraction increases; this decrease is a result of the increasing average gas temperature for the single-region model and the increasing high-temperature product gas volume fraction for the two-region model. However, the venting rate for the two-region model decreases less rapidly in the early stages of the burn since the venting rate for the portion of the tank still occupied by reactant gas is calculated at the reactant gas temperature. The two-region venting rate is approximately 50% greater than that calculated with the single-region model for product gas volume fractions between 0.2 and 0.7. The venting rate for the two-region model decreases more rapidly towards the end of the burn. Equation (C18) gives a two-region to single-region venting rate ratio of 1.37 for these product and reactant gas temperatures (assuming a constant flame front speed). The radiative heat rate for both models increases as the product gas volume fraction increases. However, the radiative heat rate for the two-region model increases much more rapidly in the early stages of the burn due to the contribution from the hot product gas. The two-region radiative heat rate is at least an order of magnitude greater than that calculated with the single-region model for product gas volume fractions below approximately 0.4. The radiative heat rate for the two-region model increases less rapidly towards the end of the burn. Equation (C19) gives a two-region to single-region radiative heat rate ratio of 2.25 for these product and reactant gas temperatures (assuming a constant flame front speed).

Table C2 gives the ratio of the two-region to single-region venting and radiative heat transfer rates for a range of product and reactant gas temperatures calculated using eqns. (C18) and (C19). As shown in the table, the values calculated with a two-region model will be significantly higher than those calculated with a single-region model for all cases of interest.

The comparisons discussed above neglect a number of phenomena which would affect the relative venting and radiative heat transfer rates calculated with the single- and two-region models. The most important of these phenomena are discussed below:

Flame Front Velocity: The flame front velocity for the single-region model is constant so that the reactant and product gas volume fractions are linear with burn time; this is consistent with the averaging approach used to derive eqns. (C14) and (C15). However, with the two-region model, the flame front velocity decreases throughout the burn so that the volume fractions are not linear with burn time; the average product gas volume fraction for a waste tank deflagration would be on the order of 0.65 (Thomas 1993). As a result, the average venting and radiative heat transfer rates will be skewed towards the higher product gas volume fractions. Relative to the average values shown in Table C1, this will markedly increase the average radiative heat transfer rate for the two-region model and slightly decrease the venting rate.

Combustion Rate: The volumetric combustion rate was taken to be a constant in this analyses. However, the two-region model accounts for compression of the reactant gas so that the mass consumed per unit time, and hence the energy release rate, continually increases throughout the burn. Conversely, the energy release rate is a constant for the single-region model; the pressure will therefore increase faster in the initial stages of the burn with the single-region model. One implication of this is that the vents will be predicted to open earlier with the single-region model so that, although the venting rate may be lower, the single-region model may yield larger total mass losses by venting since the total vent time is longer.

Total Energy Release: The single-region model will vent a higher proportion of reactant gas than the two-region model over the course of the burn since average product gas volume fraction for the two-region model is greater than 0.5. The total energy released via combustion will therefore be slightly lower with the single-region model.

Emittance Value: Since the single-region model uses an average gas temperature, the emittance value assigned to the gas will be higher than that used with a two-region model [gas emittance increases as temperature decreases (Thomas 1993)]. The relative radiative heat transfer rate for the single-region model would therefore be larger than indicated in Table C1.

Reactant Gas Temperature: The two-region model accounts for heating of the reactant gas due to compression, whereas this effect cannot be accounted for with the single-region model. The relative venting rate calculated with the two-region model would therefore be smaller than indicated in Table C1.

Product Gas Temperature: The values given in Tables C1 and C2 were developed using a fixed product gas temperature for both models. However, since the venting and radiative heat rates for the two-region model are larger, the product gas temperature would be lower with the two-region model. This would decrease both the relative venting and radiative heat rates calculated with the two-region model.

The simplified quantitative comparison presented above indicates that a two-region model will give vent rates which are up to 40% larger than those calculated with a single-region model, and radiative heat transfer rates which are larger by approximately a factor of two. As discussed above, this is a simplified comparison and the actual relationship between the venting and radiative heat transfer rates calculated with these models is more complex.

Table C1 Normalized Venting & Radiative Heat Rates vs. Volume Fraction.

Product Gas Volume Fraction	Reactant Gas Volume Fraction	Average Gas Temp. (K)	Normalized Vent Rate			Normalized Radiative Heat Rate		
			Single- Region Rate	Two- Region Rate	Two-Reg./ Single-Reg. Ratio	Single- Region Rate	Two- Region Rate	Two-Reg./ Single-Reg. Ratio
0.00	1.00	300	0.058	0.058	1.00	8.1E+09	8.1E+09	1.00
0.10	0.90	570	0.042	0.054	1.28	1.1E+11	8.1E+12	76.8
0.20	0.80	840	0.035	0.050	1.44	5.0E+11	1.6E+13	32.6
0.30	0.70	1110	0.030	0.046	1.53	1.5E+12	2.4E+13	16.0
0.40	0.60	1380	0.027	0.042	1.56	3.6E+12	3.2E+13	8.93
0.50	0.50	1650	0.025	0.038	1.54	7.4E+12	4.1E+13	5.46
0.60	0.40	1920	0.023	0.034	1.49	1.4E+13	4.9E+13	3.58
0.70	0.30	2190	0.021	0.030	1.41	2.3E+13	5.7E+13	2.47
0.80	0.20	2460	0.020	0.026	1.30	3.7E+13	6.5E+13	1.77
0.90	0.10	2730	0.019	0.022	1.16	5.6E+13	7.3E+13	1.31
1.00	0.00	3000	0.018	0.018	1.00	8.1E+13	8.1E+13	1.00

Table C2 Single- vs. Two-Region Radiative Heat Transfer Rates.

Product Gas Temp. (K)	Two/Single Region Vent Rate Ratio				Two/Single Region Radiative Heat Rate Ratio			
	Reactant Gas Temp. (K)				Reactant Gas Temp. (K)			
	300	400	500	600	300	400	500	600
1500	1.17	1.11	1.08	1.05	2.00	1.83	1.67	1.50
1750	1.21	1.14	1.10	1.07	2.07	1.93	1.79	1.64
2000	1.24	1.17	1.13	1.09	2.13	2.00	1.88	1.75
2250	1.28	1.20	1.15	1.11	2.17	2.06	1.94	1.83
2500	1.31	1.23	1.17	1.13	2.20	2.10	2.00	1.90
2750	1.34	1.25	1.19	1.15	2.23	2.14	2.05	1.95
3000	1.37	1.28	1.21	1.17	2.25	2.17	2.08	2.00

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