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Simple Transient Calculations of Cell Flammable Gas Concentrations

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Abstract

The Saltstone Facility at Savannah River Site (SRS) mixes low-level radiological liquid waste with grout for permanent disposal as cement in vault cells. The grout mixture is poured into each cell in approximately 17 batches (8 to 10 hours duration). The grout mixture contains ten flammable gases of concern that are released from the mixture into the cell. Prior to operations, simple parametric transient calculations were performed to develop batch parameters (including schedule of batch pours) to support operational efficiency while ensuring that a flammable gas mixture does not develop in the cell vapor space. The analysis demonstrated that a nonflammable vapor space environment can be achieved, with workable operational constraints, without crediting the ventilation flow as a safety system control. Isopar L was identified as the primary flammable gas of concern. The transient calculations balanced inflows of the flammable gases into the vapor space with credited outflows of diurnal breathing through vent holes and displacement from new grout pours and gases generated. Other important features of the analyses included identifying conditions that inhibited a well-mixed vapor space, the expected frequency and duration of such conditions, and the estimated level of stratification that could develop.

Introduction

The Saltstone Facility receives low level liquid waste to be mixed with grout for permanent disposal as concrete in preexisting vaults. Hydrogen, Isopar L, benzene, ammonia, butanol, isopropanol, methanol, toluene, xylene, and Norpar 13 may be released from the incoming grout. These gases may form a flammable mixture in the vapor space of a vault into which grout has been poured. The purpose of this analysis is to evaluate the flammability of the vault vapor space assuming various gases emanate from the grout and assuming several different pour schedules. Calculations are performed to determine the allowed concentration in salt solution of one of the flammable gases, Isopar L, to reach the Composite Lower Flammability Limit (CLFL) at a maximum fill height of 7.3 m (24 ft). Because the gases evolve from the grout at different rates, the calculations must consider the CLFL over a period of many days. The transient calculations have a key assumption that the gases are well-mixed in the vapor space above the grout surface. A mixing calculation was completed to show that the gases would be well-mixed for most conditions. A transient diffusion calculation was completed to show the gas mixture would not reach CLFL for the times during which mixing is not expected. Only a portion of the results are provided in this paper. The original work is documented elsewhere[1,2,3].

Analysis

Four cases for different pouring schedules and gas releases are discussed in this paper. Details for the cases are presented elsewhere[1]. The release of Isopar L is strongly dependent on temperature. The temperature of grout is assumed to be a maximum of 45°C during the pour, but may reach temperatures as high as 85 to 95°C as the grout cures. The daily assumed release of Isopar L is based on experimental data taken at different temperatures. The nominal case assumes 22% of the Isopar L in the grout is released daily and that the pour schedule is for eight hours, Monday through Thursday. The bounding case assumes 92% of the Isopar L in the grout is released daily. The nominal case uses nominal values for many input parameters and is intended to illustrate the inherent margin compared to the other cases. Except for the nominal case, all of these calculations are done at a vapor space temperature of 65°C, a salt solution mass fraction of 0.50, and assuming the inventories and release fractions/profiles for the ten gases.[1] The release profiles in time for all cases are identical. The flammable gases released from each day's pour are assumed to be released after the pour has been completed. For some of the gases, the entire amount present in the poured grout is released on the day of the pour. For others, only a fraction is released on the first day and the remaining released on subsequent days. Hydrogen is released continuously from the entire amount of grout accumulated since the pour schedule began at a constant rate per unit grout volume. Ammonia is assumed to be present in the vapor space at a constant concentration throughout the pour (and thereafter).

Diurnal breathing from daily variations in atmospheric pressure are credited with depleting the vault vapor space of some of the flammable gas present. This depletion occurs every day, regardless of whether a pour occurs on that day.

Time release profiles for gases considered in this work are provided in Reference 1.

Assuming a delayed release of all the flammable gas released from the pour, the relationship between the volume of grout poured and the concentration of a flammable gas in the vapor space above the grout is found by solving the following equation:

$$\frac{dM}{dV_m} = \frac{1}{V_{molar}} - \frac{M}{V_T - V_{grout}} \tag{1}$$

This equation has the solution

$$C_{f,i} = \frac{A_i}{A} + \left(X_{o,i} - \frac{A_i}{A} \right) e^{-\frac{A V_{molar} V_{grout}}{V_T - V_{grout}}} \tag{2}$$

where V_T = the total vapor space volume of the cell before pouring,
$C_{f,i}$ = concentration fraction of gas i in the vapor space,
V_{molar} = volume occupied by a mole of gas,

V_{grout} = the volume of poured grout
$X_{0,i}$ = initial concentration of gas i in the cell,
A_i = the moles of gas I released from the grout, and
A = the total moles of gas released from the grout.

For the gases in this calculation, A is defined as

$$A = \sum_i A_i = A_{Iso} + A_{ben} + A_{but} + A_{tol} + A_{xy} + A_{meth} + A_{isoprop} + A_{hydro} + A_{Nor} \quad (3)$$

where A_{Iso} = moles of Isopar L released per liter of grout,
A_{ben} = moles of benzene released per liter of grout,
A_{tol} = moles of toluene released per liter of grout,
A_{xy} = moles of xylene released per liter of grout,
A_{meth} = moles of methanol released per liter of grout,
$A_{isoprop}$ = moles of isopropanol released per liter of grout,
A_{hydro} = moles of hydrogen released per liter of grout,
A_{Nor} = moles of Norpar released per liter of grout.

Equation (2) gives the concentration of gas x in the vapor space given a pour volume V_{grout}, a total pre-pour vapor space volume of V_T, and an initial concentration of X_0, assuming gases are released from the poured grout after the entire grout volume has been poured. This equation does not credit the displacement of gas from the current pour by the volume of grout in the current pour. It does credit the displacement of flammable gases present in the vapor space prior to the pour by the volume of grout in the previous pour. It also credits the displacement of gases in the vapor space by gases as they are released from the grout.

The final concentration of flammables in the vapor space after a series of daily pours can be determined by the application of Equation 2 at the end of each day and summing. This is because the displacement of gas in the vapor space by the volume of a pour does not change the concentration of gas. The final concentration can also be found by applying Equation 2 to each day’s pour, using the final concentration from the previous day’s pour as the initial concentration for the current day’s pour. The second method is the one used here because it is easily adapted to arbitrary pour schedules.

Equation 2 is used in the present analysis to model releases of most of the gases present. Hydrogen and ammonia are treated differently. Hydrogen is continuously generated by radiolysis. A constant rate per gal of salt solution is input to the model. This rate is applied to the entire grout volume poured prior to time t. The maximum concentration of ammonia in the vapor space was determined[1] to be 3.9 mg/l. The concentration of ammonia in the vapor space is held at this value throughout the analysis.

The purpose of the present evaluation is to determine the minimum concentration of Isopar L residing in the grout that gives the CLFL in the vapor space at a 7.3 m (24 ft) fill height. The calculation uses given concentrations of various additional flammable species in the poured grout. If the minimum allowed concentration of Isopar L is 11 ppm or greater, the percent CLFL reached using 11 ppm as the Isopar L concentration is determined. The contribution from each species present in the vapor space is calculated using Equation 2. The allowable Isopar L concentration is calculated using the Solver routine in Excel to maximize the fraction of CLFL reached in the vapor space as the Isopar L concentration in the grout is varied.

For a mixture of flammable gases, CLFL is determined using Le Chatelier's rule as

$$CLFL = \frac{1}{\sum\left[\frac{M_i^{mole}}{M_{tot}^{mole} LFL_i}\right]} \tag{4}$$

where LFL$_i$ is the lower flammability limit and M_i^{mole} the mole fraction of flammable gas i. M_{tot}^{mole} is the total mole fraction of flammable gas.

The LFL for a flammable gas is usually given at the reference temperature of 25 deg C. The LFL values in this work were corrected for elevated temperatures prior to combining to calculate the CLFL.

After the start of the pour schedule, gases are continuously exiting the cell vapor space because of daily variations in atmospheric pressure (diurnal breathing). The equation describing the mass of gas in the vapor space as a function of time with an initial gas mass undergoing diurnal breathing is

$$\frac{dM}{dt} = \frac{-MQ}{V_T - V_{grout}} \tag{5}$$

where M is the mass of the gas and Q is the volumetric flowrate from the vapor space due to breathing.

Equation 5 has the solution

$$\frac{M(t)}{M_o} = e^{-\frac{Qt}{V - V_{grout_T}}} \tag{6}$$

where M$_0$ is the mass residing initially in the vapor space.

Reference 1 uses

$$Q = 4\left(\frac{\Delta P}{P_0}\right)\left(\frac{V - V_{grout}}{t_{AB}}\right) \tag{7}$$

where ΔP is the daily variation in pressure determined from statistical analysis of 5 years of regional measured data, P$_0$ is atmospheric pressure, and t$_{AB}$ is 24 hours.

Combining equations (6) and (7) gives

$$\frac{M(t)}{M_o} = e^{-\frac{4\Delta P t}{P_0 t_{AB}}} \tag{8}$$

With $\Delta P = 2.5$ mbar, $P_0 = 1013.25$ bar, $t_{AB} = 24$ hr and t = 12 hr (the period of exhale),

$$\frac{M(t)}{M_o} = 0.995076 \tag{9}$$

Equation 9 provides the fraction of the inventory remaining in the vapor space each day after diurnal breathing.

The foregoing methodology has been implemented in an Excel spreadsheet. Table 1 summarizes the treatment of each of the flammable gases present.

Table 1. Modeling Details for Constituents.

Component	Amount in Premix	Amount in Salt Solution	Generation Rate	How treated
Isopar	N/A	TBD ppm	N/A	Time release
Ammonia	N/A	N/A	N/A	Constant concentration
Butanol	N/A	1.03 mg/l	N/A	Instant release
Isopropanol	N/A	0.25 mg/l	N/A	Instant release.
Benzene	1.607 kg in full cell	4.15 kg in full cell	N/A	Time release (two profiles)
Toluene	2.06 kg in full cell	N/A	N/A	Time release
Xylene	10% of toluene inventory	79.5 g/hr of pour	N/A	Time release
Norpar	N/A	0.1 mg/l	N/A	Instant release
Methanol	N/A	0.25 mg/l	N/A	Instant release
Hydrogen	N/A	N/A	5.59E-08 (ft3/hr/gal SS at 95 deg C)	Continuous release

In order to demonstrate that the vapor space is well-mixed, it must be shown that a stratification layer of gas or VOC will not form on the surface of the grout. This is possible when the release rate to the surface of the substance can be removed by natural convection at a rate that prevents the substance from accumulating on the surface. In other words, the mass flux due to convection must be greater than the mass flux of the substance released from the surface of the grout.

$$j_{conv} > j_{groutsurface} \tag{10}$$

where j_{conv} = mass flux due to convection, kg/(m^2-s)
$j_{groutsurface}$ = mass flux due to the substance release from the grout surface, kg/(m^2-s)

It is assumed for the mixing analysis that all the gas generated in the volume of a specified grout pour depth is released to the surface over the time of the pour. The mass flux of the substance release from the grout surface ($j_{substance}$) is related to the substance generation rate by

$$j_{substance} = R_{substance} d \tag{11}$$

where $R_{substance}$ = substance generation rate^2, kg/(m^3-s)

d = grout depth, m

The convective mass flux is calculated from

$$j_{conv} = h_D(C_1 - C_2) \tag{12}$$

where h_D = mass transfer coefficient, m/s
C_1= substance concentration at surface, kg/m^3
C_2= substance concentration in cell vapor space, kg/m^3

The mass flux is similar to the heat flux as the former is proportional to the concentration difference between two locations while the latter is proportional to the temperature difference. The proportionality constants are the mass transfer coefficient and the heat transfer coefficient.

When both heat and mass transfer are occurring simultaneously, the mass and heat transfer coefficient are related by

$$\frac{h}{h_D} = \rho c_p \left(\frac{Sc}{Pr}\right)^{2/3} = \rho c_p \left(\frac{\alpha}{D}\right)^{2/3} \tag{13}$$

where h = heat transfer coefficient, W/(m^2-K)
h_D = mass transfer coefficient, m/s
ρ = air density, kg/m^3
c_p = air specific heat at constant pressure, J/(kg-K)
Sc = Schmidt number = ν/D
Pr = Prandtl number = ν/α
ν = air kinematic viscosity, m^2/s
D = diffusion coefficient in air, m^2/s
α = air thermal diffusivity, m^2/s

Equation 13 can be solved for the mass transfer coefficient:

$$h_D = \frac{h}{\rho c_p \left(\frac{\alpha}{D}\right)^{2/3}} \tag{14}$$

The air density as a function of temperature can be obtained from the perfect gas law:

$$\rho = \frac{P}{R_a T} = \frac{P}{\left(\frac{R_g}{MW_a}\right) T} \tag{15}$$

where P = pressure in the cell vapor space, which is at atmospheric pressure, 1.01325 x 10^5 Pa
R_a = gas constant for air, J / (kg - K)
R_g = universal gas constant, 8314 kg-m^2 / (sec^2 – kg – mole - K)
MW_a = molecular weight of air, 28.97 kg / (kg-mole)
T = temperature, K

The heat transfer coefficient is evaluated by using the equation for turbulent, free convection from a heated plate (i.e., solid surface) facing upward.

$$h = 1.52 \Delta T^{1/3} \tag{16}$$

where $\Delta T = T_s - T_r$, K
h = heat transfer coefficient, W / (m^2 – K)

The substance release rate at the surface of the grout is limited by the vapor pressure (P_v) of the substance which is a function of temperature[2]. It is assumed that all the substance produced in the grout is immediately released into the vapor space.

The concentration difference in Equation 12 is calculated from

$$\Delta C = C_1 - C_2 = \frac{P_v - P_c}{\left(\frac{R_g T_{av}}{MW_b}\right)} \tag{17}$$

where P_c = substance partial pressure in the cell vapor space, Pa
MW = substance molecular weight, kg/kg-mole

The partial pressure of the substance in the cell vapor space is obtained by multiplying the substance concentration by the atmospheric pressure (1.01325 x 10^5 Pa).

$$P_c = y_{substnace} P \tag{18}$$

The substance concentration is assumed to be the LFL value for the substance.

Equation 17 can then be solved for the concentration difference, which is then used to determine the convective mass flux from Equation 12.

The convective mass flux is then compared to the substance mass flux from the surface to determine if Equation 10 is satisfied. If the convective mass flux is greater than the substance mass flux, then no stratification occurs, and the vapor space will be well-mixed.

Initially, the calculations assumed very conservative conditions. The temperature difference between the grout surface and the roof of the cell is set to 0.1° K. The smaller this temperature difference, the more difficult it is to show that mixing can occur. If the temperature difference is zero or less, the calculation cannot be completed. The reason is if the grout temperature is less than or equal to the roof temperature, no heat transfer can occur. With no heat transfer, there is no mass transfer in the heat and mass transfer analogy.

Analysis of historical temperature data showed that periods of up to 12 hours were possible on hot summer days in which cell roof temperatures can exceed the grout surface temperature, and temperature-driven natural circulation cannot be assumed to be available for mixing. Without the well-mixed condition, non-uniform flammable gas distributions would need to be considered with the potential of localized pockets of vapor space existing at above CLFL conditions even though the average flammable gas concentrations represent below CLFL conditions. Additional calculations were performed to show the level of stratification under these conditions would not be sufficient for CLFL conditions to be exceeded. For each substance, two calculations are completed for average temperatures of 50° C and 65° C. Typically as the average temperature increases, the larger the difference between the convective mixing term, j_{conv}, and the mass flux from the grout surface, $j_{groutsurface}$, in Equation 10.

A third parameter important in the calculations is the depth of the grout pour. The maximum grout depth in the cell is 7.6 m (25 ft), and the current plans are to complete the grout pouring over 21 pours. Thus, a daily grout depth can be approximated as 0.4 m (1.2 ft). Because of variations in the daily pour schedule, the daily pour depth can vary around this nominal value. The initial calculations made the very conservative assumption that the grout was completely poured in one step. This assumption results in the maximum substance generation from the grout over the shortest time frame. The maximum substance generation rate in turn places the greatest stress on the ability of the heat-mass transfer model to show that convective mixing occurs.

The one-dimensional diffusion equation in the cell vapor space is given by

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{19}$$

The cell vapor space is initially at a uniform concentration for each flammable gas. The boundary conditions are represented by a constant flux at the grout surface and a zero flux condition at the top of the vapor space. This problem can be solved by separation of variables. The following series solution for the transient concentration profile for a finite region is given in Reference 4.

$$C(x,t) - C_o = \frac{\phi L}{D}\left\{\tau + \frac{3x^2 - L^2}{6L^2} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\left[\frac{(-1)^n}{n^2} e^{-n^2\pi^2\tau}\cos\left(\frac{n\pi x}{L}\right)\right]\right\} \tag{20}$$

where C = concentration, moles/m^3

C_o = initial, uniform vapor space concentrations, moles/m^3

x = distance, m

t = time, s

ϕ = flux (at surface $x = L$), moles/m^2/s

L = finite region length, m

D = diffusion coefficient, m^2/s

$\tau = D \cdot t / L^2$

Equation 20 is solved for each flammable gas surface concentration, $C_i(L,t)$, and the results summed to determine the total concentration of the flammable gases at the surface, $C_{fg}(L,t)$.

Surface concentrations at 18 hours (64,800 s) are evaluated to conservatively bound the 12 hours, based on analysis of historical data, in which cell roof temperatures can exceed the grout surface temperature.

The initial concentration for each flammable gas ($C_{i,o}$ [moles i/m^3]) is based on the initial vapor space molar fraction ($Y_{i,o}$ [moles i/moles]).

$$C_{i,o}\,[moles\ i/m^3] = \frac{Y_{i,o}[moles\,i/moles]}{V_{mole}\,[L/mole]\times 0.001[m^3/L]} \tag{21}$$

The flux term for each flammable gas (ϕ_i) represents the release rate from the grout surface per unit area. It is determined from

$$\phi_i[moles/m^2/s] = \frac{f_i \times \rho_i[mole/L] \times V_{nom}[m^3] \times 1000[L/m^3]}{A[m^2] \times \Delta t_i[s]} = \frac{f_i \times \rho_i[mole/L] \times d_{nom}[m] \times 1000[L/m^3]}{\Delta t_i[s]} \tag{22}$$

The output surface concentration of each flammable gas is multiplied by the molar volume (V_{mole}) to get the mole fraction of each flammable gas (Y_i). Similarly, the total concentration of the flammable gases at the surface is multiplied by the molar volume (V_{mole}) to get the total mole fraction of flammable gases (Y_{tot}).

$$Y_i\ [\text{moles i/moles}] = C_i(L,t)\ [\text{moles i/m}^3] \times V_{mole}\ [\text{L/mole}] \times 0.001\ [\text{m}^3/\text{L}] \tag{23}$$

$$Y_{fg}\ [\text{moles fg/moles}] = C_{fg}(L,t)\ [\text{moles fg/m}^3] \times V_{mole}\ [\text{L/mole}] \times 0.001\ [\text{m}^3/\text{L}] \tag{24}$$

The total mole fraction of flammable gases is compared to the CLFL to determine if a flammable mixture is present at the surface.

The CLFL is determined using Le Chatelier's rule (Equation 4).

An important aspect of the calculations is to correctly account for temperature dependencies. The LFL and mass transfer diffusivity for each flammable gas is corrected for temperature while the molar volume is corrected for temperature using the volume-temperature relationship from the ideal-gas law.

Results

The limiting Isopar L results[1] are given in Table 2.

Additional cases determined the effect of delayed Isopar L releases. The same Isopar L release profile as a function of time that was used for the results in Table 2 was used for the results in Table 3 for different Isopar L delays. Other parameters were fixed at the values used in Case 3 (4/3 pour schedule). The results are shown in the following table:

For comparison, the Case 2 results, which do not assume a delay, are 13.00 ppm to reach 100% CLFL and 89.83% CLFL assuming 11 ppm. It can be concluded that allowed Isopar L concentrations and percents to CLFL resulting from uniform delays up to three days using the Case 3 release fraction vs. height profile are bounded by those using the constant 92% release fraction and no delay. While not all pour layers are expected to experience the same delay, it is judged that the conservatism inherent in the assumption of a constant 92% release fraction compensates for uncertainty in the timing of releases from poured grout.

Table 4 shows that convective mixing occurs for conservative grout pours. In Table 9, no convective mixing occurs for three temperature cases. For these cases, the vapor pressure of Norpar 13 and Isopar L is lower than the LFL. Thus for these cases, there is no LFL concern.

Table 2. Summary of Results.

Case	Isopar L Release Fraction	Pour Schedule	Allowable Isopar L Concentration in Salt Solution at 24 ft, (ppm)	Fraction of CLFL with 11 ppm Isopar L in Salt Solution (%)
1	Height (m) Fraction (%) 0-0.5 92 0.5-6.5 92 > 6.5 92	10 hr pours on days 1-5, 8, 15, 22, 29, 33, 41, 48, 54, 60, 67, 74, 80.	15.09	81.11
2	Height (m) Fraction (%) 0-0.5 92 0.5-6.5 92 > 6.5 92	8 hr Mon-Thurs	13.00	89.83
3	Height (m) Fraction (%) 0-0.5 22 0.5-6.5 92 > 6.5 22	10 hr every day	12.83	91.14
		8 hr every day	15.10	82.81
		8 hr every other day	17.56	75.02
		8 hr Mon-Thurs	17.00	76.58
Nominal	Height (m) Fraction (%) 0-0.5 22 0.5-6.5 22 > 6.5 22	8 hr Mon-Thurs	82.18	34.06

Table 3. The Effect of Delayed Isopar Releases.

Isopar L Release Delay (days)	Allowable Isopar L Concentration in Salt Solution at 24 ft, (ppm)	Fraction of CLFL with 11 ppm Isopar L in Salt Solution, (%)
0	17.00	76.58
1	15.34	81.29
2	13.90	86.22
3	13.11	89.40
4	12.73	91.08

Table 5 shows that the CLFL is not reached at the grout surface at a time of 18 hours. As one progresses through the pour schedule, the fraction of CLFL at the grout surface increases and reaches a maximum at day 56. As shown in the table, the ratios of "gas volume sum" to CLFL at Day 100 and Day 150 are lower.

Table 4. Parameters for Convective Mixing Calculations.

Substance	Grout Pour Depth, ft	Mixing at Average Temperature	
		@ 50^{o} C	@ 65^{o} C
Hydrogen	25	Yes	Yes
Ammonia	25	Yes	Yes
Butanol	4.2	Yes	Yes
Methanol	25	Yes	Yes
Benzene	25	Yes	Yes
Isopropanol	25	Yes	Yes
Toluene	25	Yes	Yes
Xylene	25	Yes	Yes
Isopar L	25	Partial pressure is less than the LFL. No mixing occurs, but no flammable mixture can exist.	Yes
Norpar 13	NA	Partial pressure is less than the LFL. No mixing occurs, but no flammable mixture can exist.	

Table 5. Fraction of CLFL for Flammable Gases at Grout Surface at 18 Hours.

Day	CLFL	Sum of Gas Volume Fractions	Satisfy CLFL	Volume Fractions / CLFL
1	6.30E-02	7.37E-03	Yes	0.12
5	6.10E-02	6.97E-03	Yes	0.11
9	2.92E-02	8.65E-03	Yes	0.30
13	4.16E-02	7.59E-03	Yes	0.18
17	2.36E-02	9.63E-03	Yes	0.41
21	2.92E-02	8.55E-03	Yes	0.29
25	1.89E-02	1.13E-02	Yes	0.60
29	1.82E-02	1.18E-02	Yes	0.65
33	1.79E-02	1.24E-02	Yes	0.69
37	1.79E-02	1.28E-02	Yes	0.72
41	1.79E-02	1.33E-02	Yes	0.74
45	1.80E-02	1.36E-02	Yes	0.76
49	1.81E-02	1.38E-02	Yes	0.76
56	1.85E-02	1.42E-02	Yes	0.77
100	2.12E-02	1.56E-02	Yes	0.74
150	2.42E-02	1.66E-02	Yes	0.69

Notes:
1. The results are given for the grout surface.
2. The "yes" in the column labeled "Satisfy CLFL" indicates that the flammable gas volume sum is less than the CLFL.
3. The last column shows the fraction of CLFL at the grout surface.

Once the grout has cured and heat generation has ceased after the last grout layer has been poured, the only significant volatile which could potentially present a flammability concern is hydrogen. However, hydrogen is lighter than air and will rapidly diffuse so that no stratification can occur and therefore natural convection is not required. Atmospheric breathing continues throughout this period removing residual flammable gases.

Conclusions

The most conservative case analyzed (10 hr every day pour schedule and 22%/92%/22% Isopar L release) results in an allowed Isopar L concentration of 12.83 ppm. This schedule is unrealistically aggressive to fill a cell but may be realistic for a portion of a fill. All other, more realistic, cases result in greater allowed Isopar L concentrations.

Convective mixing was evaluated for 50°C and 65°C conditions within a cell of Vault 4 of the Saltstone facility. The results from the analytical method indicate that convective mixing increases with increasing temperature. Convective mixing occurs for hydrogen, ammonia, butanol, methanol, benzene, isopropanol, toluene, and xylene for the 50°C and 65°C temperatures. There is no mixing for Norpar 13 but the partial pressure of Norpar 13 does not reach the LFL pressure. Thus, no explosive concentration can occur for Norpar 13. Convective mixing occurs for the higher temperature for Isopar L while the lower temperature case has a partial pressure lower than the LFL pressure, resulting in a non-explosive mixture.

Molecular diffusion is adequate to prevent the combination of hydrogen, Isopar L, benzene, ammonia, butanol, isopropanol, methanol, toluene, xylene, and Norpar 13 gases from reaching CLFL conditions for 18 hours after the loss of convective mixing in a Vault 4 cell of the Saltstone facility.

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