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Flammable Gas Concentrations In Ex-Tank Volumes

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Abstract: A simple two-volume model was defined and used for calculating flammable gas concentrations within headspace volumes of single-shell tanks, and within smaller ex-tank volumes connected to the headspace. Assumptions and parameters used to characterize the headspace portion of the model were taken from the "GRE Analysis Tool" (AT) for simulating gas release events. Additional assumptions used to construct the ex-tank portion of the two-volume model were conservative extensions of those made within the AT, and chosen to simulate headspace to ex-tank gas-flow conditions that would maximize ex-tank concentrations.

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FLAMMABLE GAS CONCENTRATIONS
IN
EX-TANK VOLUMES

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June 1998

ABSTRACT

A simple two-volume model was defined and used for calculating flammable gas concentrations within headspace volumes (V_1) of Single-Shell tanks (SSTs), and within smaller above-tank volumes (V_2) connected to the SST headspace. Assumptions and model parameters used to characterize the headspace portion of the model were taken from the "GRE Analysis Tool" (AT) for simulating gas release events (Slezak 1997a, Slezak 1997b). Additional assumptions used to construct the ex-tank portion of the two-volume model were conservative extensions of those made within the AT, and chosen to simulate V_1 - V_2 gas-flow conditions that would maximize ex-tank concentrations.

Numerical evaluations of the two-volume model were performed over a range of headspace GRE conditions and representative ex-tank parameters. To assure consistency with the AT, the range of headspace parameters was taken from 1000 simulated GREs generated by the AT computer code RESOLVE. Based upon waste level fill factors, three tanks (TX-102, SX-103, and TX-112) were chosen to represent typical large, medium, and small headspace volumes available in actual SSTs. Engineering drawings of these tanks were used to determine values of their ex-tank parameters (V_2 's and estimates for the gas-flow fraction "a" into the specific V_2). The results of these evaluations were used to compare time periods for which flammable gas concentrations in the tank headspace and the ex-tank volumes exceeded the lower flammability limit for upward flame propagation (LFL_u). These results indicate that even for relatively small flow fractions, headspace concentrations that exceed the LFL_u can cause delayed ex-tank concentrations to also exceed the LFL_u . The extent to which this occurs is determined mostly by the geometrical aspects of the model, as expressed in the effective volume fraction parameter, $V_2/(aV_1)$.

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1.0 BACKGROUND

General Context

The work reported in this document was performed in support of a larger effort being carried out by the Flammable Gas Project (FGP) office of Duke Engineering and Services Hanford (DESH) for resolving flammable gas Unresolved Safety Questions (USQ). As a integral part of this USQ closure effort, DESH has developed a technical assessment procedure called the Analysis Tool (AT) (Slezak 1997a, Slezak 1997b) to estimate possible consequences that may result from Gas Release Events (GRE) in both single and double-shell tanks.

To be consistent with the AT, all assumptions and input parameter values relevant to the analysis described in this report were taken from Slezak 1997a, Slezak 1997b, and references therein. Those assumptions and input values are treated as having been validated within the AT document, and unless otherwise stated, they will not be further discussed in this document. Also note that the specific analysis objectives and the methods used to attain those objectives were developed with frequent discussions and directions from the appropriate representatives appointed by DESH.

Specific Issue

Within the above context, the Specialty Engineering Group of FDNW was requested by DESH to provide independent technical calculations that would help determine the accident frequencies and consequences from ignition of flammable gas in ex-tank volumes connected to the dome space of single shell tanks (SSTs). These calculations were to be performed for both passive and active types of ventilation systems used currently to control the concentration of flammable gas in the headspace of the 149 SSTs. Because the active ventilation systems are subject to possible failure (from power outages, etc.), calculations for those systems were to include cases of normal and failed system operations.

2.0 OBJECTIVES

The main purpose of this analysis was to provide quantitative results to help determine frequencies of potentially hazardous flammable gas conditions within ex-tank volumes. This was accomplished by constructing simple, conservative mathematical models that related ex-tank flammable gas concentrations to headspace concentrations for passively and actively vented tanks. The models were evaluated for a range of realistic input parameters, and ratios of the ex-tank to headspace concentrations were used to estimate the relative "times at risk" (the time periods for which the flammable gas concentration exceeds the lower flammability limit for upward flame propagation [LFL_u]). This report provides a description of these models and presents numerical results for ex-tank flammable gas concentrations and relative times at risk (referred to in this report as time-at-risk ratios or TaRRs).

The material in this report is organized as follows: Descriptions of the models, including the assumptions, equations, and the choices of representative tanks whose data would be used in subsequent calculations are given in the METHODS section. Specific numerical values for the model input and the resulting output are given and discussed in the RESULTS section, which for the purpose of clarity in presentation includes only the main numerical results. Execution of all intermediate parameter evaluation procedures and corresponding results are included in the APPENDIX section.

3.0 METHODS

In this section, the detailed model assumptions, equations, and evaluation procedures are presented for the Passive Ventilation and Active Ventilation cases separately. Before these separate cases are discussed, however, the base assumptions common to both cases are first listed in subsection 3.1. The discussions for the separate cases are then given in subsections 3.2 and 3.3, in which the additional assumptions, equations, and solutions are delineated for the Passive and Active cases respectively. The numerical evaluation, and input selection procedures are the same for both cases, and are specified in subsection 3.4. To attain the main objectives of this analysis in a manner consistent with the AT model, all assumptions and parameters used to calculate headspace and (when appropriate) ex-tank concentrations and times at risk were taken directly from the AT-RESOLVE computer code.

3.1 BASE ASSUMPTIONS

The assumptions listed in the following four categories establish the general framework for the ex-tank models used in this report. The statements given in the first two categories are essentially recapitulations of the assumptions used in the AT procedures that were relevant to this report's objectives. Similarly, the statements in the first half of the third category (headspace Well-Mixed Concentrations) were also taken from the AT. The assumptions listed in the second half of the third, and all of the fourth categories are new and apply to the ex-tank volumes under consideration.

- Natural Circulation & Initial Headspace Conditions

Gas-flow patterns within the headspace have been extensively studied and are driven by the temperature difference between the relatively warm waste surface and the cooler surroundings (for example, see Antoniuk 1997 and references therein). This temperature-driven "natural circulation" within the headspace is a stable, torus-shaped flow pattern. The effects of fluctuations in the ambient barometric pressure have been considered (by using the barometric breathing rates given in Crippen 1993) and were found to be negligible (about 3% to 5%) compared to total passive ventilation rates (given in Stauffer 1997). Thus, natural circulation is assumed to be the dominant baseline gas flow into which localized concentrations of flammable gas are injected from regions of the waste surface. For the purposes of this report, it will further be assumed that the natural circulation pattern causes a constant, one directional, flow from the tank headspace through the ex-tank volume under consideration.

The amount of flammable gas injected is assumed to be relatively small, and thus does not disturb the natural circulation pattern significantly. The injection mechanism is described in terms of episodic gas release events (GRE) occurring as peaks above a constant baseline (steady-state) value. The models in this report were created to study the ex-tank response to GRE induced concentrations. Consistent with the AT, the initial concentration of flammable gas within the headspace is assumed negligible at the start of a GRE.

- GRE Modeling

The AT model uses a flammable gas release rate during a GRE that changes abruptly from a value of zero to the constant value, r_{sg} for the period of time τ_{rel} , and then back to zero. Letting $R_{GRE}(t)$ represent the GRE release rate as a function of time, the step-wise time dependence of the AT model can be written as

$$\text{Eq. 1, } R_{GRE}(t) = \begin{cases} 0 & \text{for } t \leq 0 \\ r_{sg} & \text{for } 0 < t \leq \tau_{rel} \\ 0 & \text{for } \tau_{rel} < t \end{cases}$$

consistent with the AT the specific values for r_{sg} and τ_{rel} used in this report were taken from the Resolve output files. (These values are listed in Table 2 of the Results section.)

- Well-Mixed Concentrations

As in the AT, the concentration in the headspace is assumed to be uniform throughout the entire volume. This assumption implies an instantaneous mixing of GRE gas within the headspace. For this to be valid within the models, the smallest time increments for the models must be larger than the mixing time required for the headspace to reach homogeneity after the onset of a GRE. From tracer gas measurements (Huckaby 1997), and computer modeling (Antoniak 1997) tank headspace mixing to homogeneity is expected to be completed in about one hour. Thus, the well-mixed assumption implies that the explicit time dependence all effects that vary within times less than one hour are being neglected.

In a similar manner, the gas concentrations in the ex-tank volumes will also be assumed homogeneous. Moreover, no attempt will be made to describe a time lag in the ex-tank concentrations that result from the physical distance between the headspace and the ex-tank volume. This communication time is expected to be longer than the mixing time, and in principle should be accounted for within the ex-tank model. However, it would be included as a constant shift in time between the headspace and ex-tank concentrations, but it would not affect the relative times at risk results. For the purposes of this analysis, it is thus safe to ignore this additional time-dependent effect.

- Representative Ex-Tank Parameters

To perform calculations for ex-tank models, specific values for ex-tank parameters are required. Procedures for obtaining such parameter values are not specified in the AT model, and thus must be specified herein. Based upon current headspace volumes, three tanks were chosen as representative examples of small, medium, and large SST headspace volumes. These representative tanks are TX-112 (high fill factor), SX-103 (medium fill factor), and TX-102 (low fill factor). From the appropriate engineering drawings of these tanks, possible ex-tank volumes and gas flow paths were identified and their dimensions recorded (and included in subsection 7.2 of the Appendix). These dimensions were then used to calculate the ex-tank volumes and estimate the flow fractions to each region.

3.2 PASSIVE VENTILATION MODEL

Assumptions

The basic assumption for the passive ventilation case is that the only mechanism for free exchange of gas between the SST headspace and the aboveground atmosphere (air) is via open channels other than the ex-tank region of interest (e.g., filtered ports, hatchways, etc.). As mentioned in the Base Assumptions, the ex-tank volume is assumed to be a one-way (exhaust) channel for headspace gas outflow only. All gas entering the ex-tank volume from the headspace is exhausted into the atmosphere. In this model, air flows into the headspace through some open channel and out through some other open channel and through the ex-tank region. This is a conservative assumption in that any reversal of flow direction between the headspace and the ex-tank region is ignored, thus maximizing the ex-tank flammable gas concentration for a given concentration in the headspace.

The salient features associated with the passive ventilation model are depicted in Figure 1. In this figure, the background natural circulation pattern within the headspace (V_1) is shown by the torus shaped double arrows indicating a flow upward in the center and downward along the sides of the tank. Flammable gas is injected from the waste at the rate r_{sg} . Air enters the headspace from one channel and dilutes the flammable gas concentration. The resulting well-mixed flammable gas concentration exits the headspace through the ex-tank volume (V_2) at the rate " $a r_{eff}$ ". The exit flow rate via the sum over all other possible channels is indicated as " $(1-a) r_{eff}$," where the parameter " a " represents the fixed fraction of headspace ventilation flow through V_2 . The flow direction is defined as positive outward from headspace, as indicated by the vertical arrows, and the net rate balance of flammable gas within the headspace is shown by comparing the injection rate (r_{sg}) to the sum over the exit rates (r_{eff}). To assure the flow rates do not violate mass conservation, r_{eff} is taken to be r_{sg} or if larger, the actual passive rate, r_{vent} .

Figure 1: Passive Ventilation

Equations for the Passive Ventilation Model

Within the framework of the above assumptions, the following first-order, ordinary differential equations were used to relate the headspace (Y_1) and ex-tank (Y_2) concentrations:

$$\text{Eq. 2, } V_1 \frac{dY_1(t)}{dt} = \begin{cases} N_0 r_{sg} - Y_1(t) r_{eff} & \text{for } 0 < t \leq \tau_{rel} \\ 0 - Y_1(t) r_{vent} & \text{for } \tau_{rel} < t \end{cases}$$

and

$$\text{Eq. 3, } V_2 \frac{dY_2(t)}{dt} = \begin{cases} Y_1(t) a r_{eff} - Y_2(t) a r_{eff} & \text{for } 0 < t \leq \tau_{rel} \\ Y_1(t) a r_{vent} - Y_2(t) a r_{vent} & \text{for } \tau_{rel} < t \end{cases}$$

Note that these equations are for GRE induced flammable gas concentrations in excess of the steady-state values, which in accord with the base assumption are taken as zero, i.e. $Y_1(t) = Y_2(t) = 0$ for $t \leq 0$ and in the limit $t \rightarrow \infty$. Also note that Eq. 2 is identical in form to the one-volume AT model, and that the GRE source term in this equation was obtained by multiplying the GRE concentration (N_0) times the release rate given in Eq. 1. For completeness, the definitions and dimensions for all the symbols used in the above equations are listed below.

Table 1 : Mathematical Symbol Definitions

SYMBOL	DEFINITION	UNITS
$Y_1(t)$	tank headspace flammable gas concentration	(molar fraction)
$Y_2(t)$	ex-tank volume flammable gas concentration	(molar fraction)
τ_{rel}	GRE duration	(seconds)
N_0	GRE flammable gas concentration	(molar fraction)
r_{sg}	GRE gas release rate	(meters ³ /second)
r_{vent}	Tank ventilation rate	(meters ³ /second)
r_{eff}	The largest between r_{sg} and r_{vent}	(meters ³ /second)
V_1	Tank headspace volume	(meters ³)
V_2	Ex-tank volume	(meters ³)
a	Fraction of r_{vent} flowing through V_2	(dimensionless)

Solutions

Because Eq. 2 for the in-tank concentration $Y_1(t)$ is independent of $Y_2(t)$, it can be solved independently from Eq. 3, and is easily obtained by applying standard analytic procedures for uncoupled, first-order linear differential equations of this form (Braun 1983). The following closed-form expression can be shown (upon differentiation and substitution) to satisfy Eq. 2 and the steady-state boundary conditions at $t = 0$ and $t \rightarrow \infty$:

$$\text{Eq. 4, } Y_1(t) = \begin{cases} \left(\frac{N_0 r_{sg}}{r_{eff}} \right) G_1(t) & \text{for } t \leq \tau_{rel} \\ Y_1(\tau_{rel}) D_1(t) & \text{for } t > \tau_{rel} \end{cases}$$

In this expression, the time dependence is given by the standard exponential growth (G) and decay (D) functions:

$$\text{Eq. 5, } G_1(t) = \left[1 - \exp\left(-\frac{r_{\text{eff}}}{V_1} t\right) \right] \quad \text{and} \quad D_1(t) = \exp\left(-\frac{r_{\text{vent}}}{V_1} (t - \tau_{\text{rel}})\right),$$

for which the limiting values $G_1(t=0) = D_1(t=\infty) = 0$ guarantee satisfaction of the boundary conditions. Also note that the maximum headspace growth factor is $G_1(t=\tau_{\text{rel}})$ and is used to define the constant maximum concentration, $Y_1(\tau_{\text{rel}})$, in the $t > \tau_{\text{rel}}$ part of Eq. 4.

Using the above simple closed form solution for $Y_1(t)$ and analogously defined ex-tank exponential growth and decay functions, Eq. 3 can also be solved by similar standard analytic methods, yielding the following solution:

$$\text{Eq. 6, } Y_2(t) = \begin{cases} \left[\frac{1}{(1-f_{21})} \left(\frac{N_0 r_{\text{sg}}}{r_{\text{eff}}} \right) \right] [G_1(t) - f_{21} G_2(t)] & \text{for } t \leq \tau_{\text{rel}} \\ \left[\frac{1}{(1-f_{21})} Y_1(\tau_{\text{rel}}) \right] \left[D_1(t) - f_{21} \left(\frac{G_2(\tau_{\text{rel}})}{G_1(\tau_{\text{rel}})} \right) D_2(t) \right] & \text{for } t > \tau_{\text{rel}} \end{cases},$$

where the "effective volume fraction", $f_{21} = V_2 / (aV_1)$ is used to define the reoccurring ratio of volumes, and the ratio (a/V_2) characterize the ex-tank exponents instead of the $(1/V_1)$ headspace ratio, i.e.

$$\text{Eq. 7, } G_2(t) = \left[1 - \exp\left(-\frac{ar_{\text{eff}}}{V_2} t\right) \right] \quad \text{and} \quad D_2(t) = \exp\left(-\frac{ar_{\text{vent}}}{V_2} (t - \tau_{\text{rel}})\right).$$

The ex-tank solution in Eq. 6 was written in a form similar to that of the headspace solution in Eq. 4 to isolate their different time dependencies. The use of the effective volume fraction enables the purely geometrical aspects of the solution to be separated from the dynamical features of the solution. This parameter also helps to sort numerical results from different cases into groups of similar behavior.

The above solutions (Eq. 4 and Eq. 6) form the core of the numerical analysis presented in this report. By comparing these expressions, the following general observations can be noted:

- The headspace concentration increases exponentially during the GRE, reaching a maximum value of $Y_1(\tau_{\text{rel}})$ at the termination of the GRE.
- The ex-tank concentration also increases exponentially during the GRE release, but the growth rate and maximum value attained during this time period is determined by the effective volume fraction, $f_{21} = V_2 / (aV_1)$ and the exponential growth rates (r_{eff} / V_1) and (ar_{eff} / V_2) .
- In general, the ex-tank concentration continues to increase after the GRE has terminated, and its peak time and value are also determined by the effective volume fraction and growth rates. The specific value for the ex-tank peak time (T_2) is obtained by finding the value of time for which the derivative of Eq. 6 is zero, and can be written as

$$T_2 = \tau_{\text{rel}} + \left(\frac{f_{21}}{1-f_{21}} \right) \left(\frac{V_1}{r_{\text{vent}}} \right) \ln \left[\frac{G_2(\tau_{\text{rel}})}{G_1(\tau_{\text{rel}})} \right].$$

3.3 ACTIVE VENTILATION MODEL

Assumptions

The active ventilation model is built upon the passive ventilation model by including a fan-powered (one-way) exhaust channel in addition to the other gas-exchange channels in the passive case. The ventilation rate through this additional exhaust channel was used only when larger than the passive ventilation rates, but less than the GRE supply rate, i.e. $r_{sg} > r_{vent}$. Thus during the GRE ($0 < t \leq \tau_{rel}$), the active exhaust channel reduces the effective flow rate into the ex-tank volume. After the GRE, the active vent rate dominates over the passive exhaust rate and causes a reversal of gas flow direction from the ex-tank volume back into the headspace. Note that a failure of the active ventilation system (loss of fan power) in this model is described by the passive model for the same tank.

The salient features associated with the active ventilation model are depicted in Figure 2. As in Figure 1 for the passive case, flammable gas is injected from the waste at the rate r_{sg} into the background natural circulation pattern within the headspace (V_1). Air enters the headspace through one channel and dilutes the flammable gas concentration, but now the resulting well-mixed flammable gas concentration exits the headspace through three channels: the actively vented channel (at the rate r_{vent}), the ex-tank volume (V_2 , at the rate " $a(r_{sg} - r_{vent})$ "), and all other possible channels (at the rate " $(1-a)(r_{sg} - r_{vent})$ "). Note that upon termination of the GRE ($r_{sg}=0$), the exhaust rates through the ex-tank and "all other" channels become negative, indicating a reversal of flow direction through these passive channels. This flow reversal results from the assumed dominance of the active ventilation rate over the passive ventilation rate, and draws flammable gas from the ex-tank volume back into the headspace.

Figure 2: Active Ventilation

Equations for the Active Ventilation Model

The inflow and outflow assumptions stated above are embodied in the following differential equations that relate the headspace (Y_1) and ex-tank (Y_2) flammable gas concentrations for the active ventilation case:

$$\text{Eq. 8, } V_1 \frac{dY_1(t)}{dt} = \begin{cases} N_0 r_{sg} - Y_1(t) r_{sg} & \text{for } 0 < t \leq \tau_{rel} \\ Y_2(t) a r_{vent} - Y_1(t) r_{vent} & \text{for } \tau_{rel} < t \end{cases}$$

and

$$\text{Eq. 9, } V_2 \frac{dY_2(t)}{dt} = \begin{cases} Y_1(t) a (r_{sg} - r_{vent}) - Y_2(t) a (r_{sg} - r_{vent}) & \text{for } 0 < t \leq \tau_{rel} \\ 0 - Y_2(t) a r_{vent} & \text{for } \tau_{rel} < t \end{cases}$$

The symbols used in these equations have the same definitions and dimensions as in the passive ventilation case (listed in Table 1), and the solutions are subject to the same boundary conditions. Note that all the coefficients in these equations are positive constants, because the only cases considered were those for which the rate of gas injection was larger than the active ventilation rate ($r_{sg} > r_{vent}$) during the GRE ($0 < t \leq \tau_{rel}$). Also note that (unlike the passive ventilation case) the headspace continues to be supplied with flammable gas after the GRE terminates as the ventilation system draws gas from the ex-tank volume back into the headspace.

Solutions

The steps for obtaining analytical solutions to Eq. 8 and Eq. 9 is somewhat different from the passive ventilation case, because the headspace concentration $Y_1(t)$ is independent of $Y_2(t)$ only during the GRE. After the GRE, it is the ex-tank concentration $Y_2(t)$ that becomes independent of $Y_1(t)$. Nevertheless, at any one time, one of the rate equations is independent of the other, thus admitting the following closed-form expressions as solutions:

$$\text{Eq. 10, } Y_1(t) = \begin{cases} N_0 G_1^{AV}(t) & \text{for } t \leq \tau_{rel} \\ Y_1(\tau_{rel}) D_1(t) + \left(\frac{a f_{21}}{1 - f_{21}} \right) Y_2(\tau_{rel}) [D_1(t) - D_2(t)] & \text{for } t > \tau_{rel} \end{cases}$$

and

$$\text{Eq. 11, } Y_2(t) = \begin{cases} \left[\frac{N_0}{\left(1 - f_{21} \left(\frac{r_{sg}}{r_{sg} - r_{vent}} \right) \right)} \right] \left[G_1^{AV}(t) - f_{21} \left(\frac{r_{sg}}{r_{sg} - r_{vent}} \right) G_2^{AV}(t) \right] & \text{for } t \leq \tau_{rel} \\ Y_2(\tau_{rel}) D_2(t) & \text{for } t > \tau_{rel} \end{cases}$$

The time dependence of these equations is given by the same growth (G) and decay (D) functions used in the passive ventilation case (Eq. 5 and Eq. 7), but with r_{eff} replaced by r_{sg} in the headspace exponential growth rate (G_1 in Eq. 5) and by $(r_{sg} - r_{vent})$ in the ex-volume growth (G_2 in Eq. 7), i.e.:

$$\text{Eq. 12,} \quad G_1^{AV}(t) = \left[1 - \exp\left(-\frac{r_{sg}}{V_1} t\right) \right] \quad \text{and} \quad G_2^{AV}(t) = \left[1 - \exp\left(-\frac{a(r_{sg} - r_{vent})}{V_2} t\right) \right].$$

Finally note that the constant concentrations $Y_1(\tau_{rel})$ and $Y_2(\tau_{rel})$ used in the $t > \tau_{rel}$ parts of these solutions are determined uniquely by evaluating the $t \leq \tau_{rel}$ parts at the upper limit. Unlike the passive case, both of these constants can be shown to be the maximum values of their respective functions. Moreover, it can be shown that at $t = \tau_{rel}$, $Y_1(\tau_{rel}) \geq Y_2(\tau_{rel})$, and for $t > \tau_{rel}$, the ex-tank decay rate is much faster than the headspace decay rate. This guarantees that after the GRE terminates, $Y_1(t) > Y_2(t)$.

3.4 INPUT SOURCES & NUMERICAL EVALUATION PROCEDURES

Numerical evaluation of the two-volume model required specific values for seven parameters: two ex-tank parameters (V_2 and "a") and five headspace parameters (V_1 , r_{vent} , N_0 , r_{sg} , and τ_{rel}). Values for the ex-tank parameters were determined from the appropriate engineering drawings for the three representative SSTs. Specific values for the ex-tank volumes (V_2) were calculated from the dimensions given in these drawings. Values for the ex-tank flow fractions (a) are affected by many factors, and could not be determined uniquely. Instead, a rough estimate of a range of values was made by considering the relative cross-sectional areas of the connecting pathways, the radial location of the pathways (with respect to the headspace natural circulation direction), and the riser diameters and blockage status. To assure consistency with the AT model, all the headspace parameters were taken directly from the AT-RESOLVE computer code output. Values of these parameters were classified as either "fixed" or "variable," as explained next.

Of the five headspace parameters taken from the AT-RESOLVE code, values for the two "physical" tank parameters (V_1 and r_{vent}) were fixed for each tank. One of the three GRE parameters (N_0) was the same for all tanks. But values for the remaining two GRE parameters (r_{sg} and τ_{rel}) were obtained by random sampling cumulative probability distribution functions (PDFs). This occurs because the AT-RESOLVE code is used to calculate GRE probabilities, with parameters obtained from expert-solicited PDFs. Thus, the specific values of these two parameters varied, depending upon the specific PDF sampling "instance." For the time-at-risk ratios (TaRRs) reported in this paper, a range of probable GRE sizes was simulated by 1000 such random sampling instances.

The numerical evaluation of the two-volume model equations was performed with the computer code EXTANK, which was written specifically to use the output from the AT-RESOLVE code as input for calculating the TaRRs for the full (1000 instance) simulation. Output from EXTANK was verified against hand and spreadsheet calculations. For the passive ventilation (uncoupled) case, EXTANK was also verified against AT-RESOLVE by comparing the times at risk for the headspace concentrations only (the denominator of the TaRR calculations). A brief description and a listing of EXTANK are given in the Appendix.

To show the explicit time dependence of the headspace and ex-tank concentrations separately, spreadsheet calculations were used to evaluate the model equations for one of the (1000) simulation instances. (The Hanford Site standard spreadsheet, Microsoft EXCEL[®], was used for these calculations.)

4.0 RESULTS

In this section, specific results are shown for three of the nine examples of ex-tank volumes studied. The results for the remaining six cases are given in subsection 7.1 of the Appendix. Because the geometrical aspects of the model equations [as embodied in the effective volume fraction, $f_{21} = V_2 / (aV_1)$] tended to dominate the behavior of the solutions, cases with similar values of f_{21} gave similar results. The three cases presented in this section were chosen to represent the range of f_{21} 's studied in both the passive and active ventilation cases. Values for the complete range of input parameters and useful combinations of these parameters are listed in Table 2, as explained below.

Table 2: Input Parameter Values for Representative SSTs

Parameter	Units	TX-112	SX-103	TX-102
"Fixed" Ex-Tank Parameters				
(small) V_2	m^3	6.716	5.522	6.482
(medium) V_2	m^3	16.791	6.482	17.745
(large) V_2	m^3	19.457	11.534	24.747
Range for "a"	None	0.005 – 0.500	0.005 – 0.500	0.005 – 0.500
"Fixed" Headspace Parameters (for all 1000 simulation instances)				
V_1	m^3	1524.6	2363.34	3159.96
r_{vent} [passive]	$10^{-3} m^3/s$	0.083	4.72	0.167
r_{vent} [active]	$10^{-3} m^3/s$	N/A	23.6 (50 cfm)	N/A
N_0	None	0.75	0.75	0.75
"Variable" Headspace Parameters (listed for one simulation instance , no. 375)				
r_{sg}	m^3/s	2.893E-1	3.049E-1	8.648E-2
τ_{rel}	$10^3 s$	4.25	4.25	4.25
Useful Combinations of Parameters: Effective Vol. Fractions & Growth and Decay Rates				
(V_2/aV_1)	None	2.552 – 0.009	0.976 – 0.005	1.566 – 0.004
(r_{eff}/V_1) [passive & active]	$10^{-3} s^{-1}$	0.190	0.129	0.027
(ar_{eff}/V_2) [passive & active]	$10^{-3} s^{-1}$	0.074 – 21.5	0.132 – 27.6	0.017 – 6.67
(r_{vent}/V_1) [passive]	$10^{-8} s^{-1}$	5.44	199.7	5.29
(r_{vent}/V_1) [active]	$10^{-8} s^{-1}$	N/A	988.5	N/A
(ar_{vent}/V_2) [passive]	$10^{-6} s^{-1}$	0.0213 – 61.8	2.05 – 427.4	0.034 – 12.9
(ar_{vent}/V_2) [active]	$10^{-6} s^{-1}$	N/A	10.25 – 2,137	N/A

The information in Table 2 is divided into four sections: "Fixed" Ex-Tank Parameters, "Fixed" Headspace Parameters, "Variable" Headspace Parameters, and Useful Combinations of Parameters. The "Fixed" and "Variable" labels distinguish between groups of parameters that

remain fixed or vary as a function of the GRE (randomly sampled) simulation instance. The top section of this table gives the complete set of nine ex-tank volumes and range of gas flow fractions studied. The detailed information used to set these values is given in the Appendix, section 7.2. The values of the headspace parameters listed in the second and third sections were taken from the AT-RESOLVE output, where the headspace volumes, ventilation rates, and flammable gas mole fractions remained fixed for all (1000) simulation instances. However, the GRE release rates and durations varied as a function of instance, and the values listed for these parameters were taken from instance no. 375. Note that the GRE flammable gas concentration parameter, N_0 , was set to a constant value of 0.75, which was the constant H_2 mole fraction used in the AT-RESOLVE calculations.

The fourth section of Table 2 gives values for the effective volume fractions, $f_{21} = (V_2 / aV_1)$, and exponential growth and decay rates. These combinations of input parameters govern the behavior of the model solutions (Eq. 6, Eq. 7, Eq. 10, and Eq. 11), and are used to describe the numerical results obtained for the values listed in the preceding sections. Entries in this section of the table that appear as ranges are for parameter combinations involving the ratio (V_2 / a) . The upper and lower limits of these value ranges were calculated from the extreme values of flow fractions ($a=0.005$ and 0.500) and ex-tank volumes (small- V_2 and large- V_2), e.g. $\text{Max}(V_2/a) = (\text{Large-}V_2)/0.005$. Note from the first row of this section that there is a large degree of overlap in the values of the f_{21} 's for the three example SSTs. Because of their dominant role in determining the behavior of the solutions, the detailed distribution of f_{21} vs. V_2 for the range of parameters studied are shown in Figure 3, below.

Figure 3: Effective Volume Fraction (f_{21}) vs. Ex-Tank Volume (V_2)

In Figure 3, 63 values of the ratio $f_{21} = (V_2 / aV_1)$ are shown as a scatter plot using three symbol types (triangles, squares, and circles), where each symbol type corresponds to one of the three SST headspace volumes (V_1). Because there are three ex-tank volumes (V_2) for each headspace volume, plots of f_{21} vs. V_2 produces nine stacks of symbols (three stacks for each SST). Each stack (or case) consists of seven identical symbols. Each symbol corresponds to one value for V_1 , one value for V_2 , and seven values for the flow fraction ($a=0.005, 0.010, 0.020, 0.050, 0.100, 0.200, \text{ and } 0.500$).

Each of the 63 values shown in Figure 3 also represents a numerical evaluation consisting of 1000 GRE simulation instances. These evaluations were used to produce the main results of this report – the time-at-risk ratios (TaRRs). From the distribution in Figure 3, note that 50 of the 63 evaluations have f_{21} values less than 0.5, where 26 of those are clustered in the $5 - 7 \text{ m}^3$ region of V_2 , and 13 are in the $16 - 20 \text{ m}^3$ region. The overlapping symbols within these regions correspond to numerical calculations that produced similar results. Thus, to show the full range of results, only three of the nine cases are presented here. The three cases selected for this purpose were the $V_2=6.48 \text{ m}^3$ ex-tank volume for TX-102, $V_2=11.5 \text{ m}^3$ for SX-103, and $V_2=19.5 \text{ m}^3$ for TX-112; chosen to represent the regions of small, medium, and large V_2 's, respectively. The time-at-risk ratios for these tanks are shown in Figure 4, Figure 5, and Figure 6, below. (For completeness, the TaRR results for the other six cases are given in subsection 7.1 of the Appendix.)

In Figures 4-6, the TaRRs for the three representative cases are plotted as a function of released-gas volumes for three values of flow fractions ($a=0.20, 0.05, \text{ and } 0.01$). Note that the scales of the axes differ for each figure because they each have different amounts of available retained gas (void fraction times total waste volume). The smallest available amount of retained gas is for TX-102 (largest headspace volume) and the largest is for TX-112. This difference in available retained gas not only affected the ranges of TaRR and GRE volumes, but also affected the number of simulation instances that qualified for TaRR evaluation (headspace concentration $\geq \text{LFL}_{\text{air}}$). Of the 1000 instances calculated by the AT-RESOLVE code, only 52 qualified for TX-102, whereas, 798 qualified for SX-103 and 982 qualified for TX-112. All 52 values for TX-102 are shown in Figure 4. To avoid unnecessary clutter in Figures 5 and 6, only 52 values of qualified instances are plotted for SX-103 and TX-112.¹⁾

Another feature seen in Figures 4-6 that results from the difference in waste (headspace) volumes is the shift of $\text{TaRR} > 0$ threshold GRE volume values. The threshold value for the $a=0.20$ TaRRs moves downward from about 170 m^3 for TX-102 to about 80 m^3 for TX-112. Similarly, but to a lesser degree, the threshold value for the $a=0.05$ TaRRs moves downward from about 190 m^3 to about 120 m^3 for these SSTs. The threshold value for the $a=0.01$ TaRRs remains roughly constant at 240 m^3 . Apparently, the shift in threshold value for the $a=0.20$ TaRRs closely follows the shift in the headspace, i.e. a high concentration of flammable gas is more easily reached as the amount of waste (headspace) is increased (decreased). For $a=0.20$ (and larger) value of flow fraction it appears that the natural circulation purging mechanism has a negligible effect. As the flow fraction decreases from $a=0.20$ to $a=0.01$, the shift in threshold values also decreases, reflecting the increasing influence of natural circulation. The constant threshold value for the $a=0.01$ flow fraction results gives a constant cross-over GRE volume of about $300 \pm 100 \text{ m}^3$ for which all TaRRs > 1 .

1) The groups of 52 values were chosen to include instance 375. This selection criteria does not prejudice the results displayed because each random sampling used by the AT-RESOLVE code to determine the GRE parameters is independent. Thus any set of 52 values represents equally the full set of TaRR values.

Figure 4: Time-at-Risk Ratio (TaRR) vs. GRE Vol. for TX-102

Figure 5: Time-at-Risk Ratio (TaRR) vs. GRE Vol. for SX-103

Figure 6: Time-at-Risk Ratio (TaRR) vs. GRE Vol. for TX-112

A final observation worth mentioning about the TaRR results can be seen in Figure 5 for SX-103. Note in this figure that the fluctuations from the otherwise apparently smooth shape of the TaRR for $a=0.01$ is a result of r_{eff} using the larger of r_{sg} or r_{vent} .

Each point in the above TaRR figures is calculated from the ratios of elapsed times for which the flammable gas concentrations exceed the LFL_a. However, these ratios do not indicate the relative values of the ex-tank and headspace concentrations. To display this dynamic aspect of the concentrations, one simulation instance (no. 375) was selected for study, and some of the results for SX-103 are shown in Figures 7 and 8, discussed next.

In Figures 7 and 8, the hydrogen concentrations in the headspace (Y_1) and in the ex-tank (Y_2) are plotted as a logarithmic function of time for the SX-103 case with ex-tank volume $V_2=11.5$ m³. The results shown in Figure 7 are the solutions for the passive ventilation model (Eq. 4 and Eq. 6), and the results in Figure 8 are the solutions for the active ventilation model (Eq. 10 and Eq. 11). The symbol key in Figure 7 applies to both figures, and indicates ex-tank concentrations for seven values of flow fraction. The $a=0.20$, 0.05, and 0.01 passive ventilation results shown in Figure 7 correspond to those used to obtain the instance 375 TaRRs shown in Figure 5.

Figure 7: H₂ Concentration vs. Time after GRE for SX-103, INST. 375 – Passive Vent. Figure 8: H₂ Concentration vs. Time after GRE for SX-103, INST. 375 - Active Vent

From the headspace concentrations (solid lines) shown in Figures 7 and 8, the termination of the GRE at $4.25\text{E}+03$ seconds is seen clearly as the cusp at the point where the smooth exponential growth curve is matched to the smooth exponential decay curve. The time at risk for the headspace is the total elapsed time for which the values of these curves exceed the LFL_{u} (horizontal dashed line). Note from the logarithmic time scale of the abscissas in Figures 7 and 8 that the decay- LFL_{u} intersection values are at least two orders of magnitude greater than the growth- LFL_{u} intersection values. Thus, a good estimate of the time at risk can be obtained by using the value of the decay- LFL_{u} intersection only. From the decay- LFL_{u} intersection points shown in Figures 7 and 8, the headspace times at risk are seen to be approximately $1.0\text{E}+06$ and $0.2\text{E}+06$ seconds for the passive and active ventilation cases, respectively.

Estimates for the ex-tank times at risk can be obtained similarly for each value of flow fraction shown in Figures 7 and 8. For the passive ventilation case, these values are seen to increase from approximately $1.0\text{E}+06$ to $1.6\text{E}+06$ seconds as the flow fraction decreases from $a=0.50$ to $a=0.005$. Dividing by the headspace time at risk value of $1.0\text{E}+06$ seconds obtained above, the time-at-risk ratios (TaRRs) for the passive case are seen to increase from 1.0 to approximately 1.6, as the flow fraction decreases from $a=0.50$ to $a=0.005$. In comparing these values to those shown for instance 375 in Figure 5, note that the TaRRs for SX-103 in Figure 5 are for flow fractions $a=0.20$, 0.05 , and 0.01 . By using the corresponding decay- LFL_{u} intersection points in Figure 7, the TaRR values for these flow fractions increase from 1.0 to approximately 1.3, as indicated in Figure 5.

Concerning the ex-tank results for active ventilation, note that within the growth regions of Figures 7 and 8, the concentrations for both the passive and active cases are identical during the GRE. In the decay regions of these figures, however, the ex-tank concentrations for the passive case continue to increase after the GRE, whereas the concentrations for the active case decrease. This clear difference in post-GRE behavior results from the purging effect of the active ventilation as it draws gas from the ex-tank volume. From the decay- LFL_{u} intersection points shown in Figure 8, the ex-tank times at risk for active ventilation range from about $6.0\text{E}+03$ to about $7.0\text{E}+04$ seconds as the flow fraction decreases from $a=0.50$ to $a=0.005$. Dividing these values by $2.0\text{E}+05$ seconds (for the active ventilation headspace time at risk noted above) gives TaRR values of approximately 0.03 to 0.35 for the range of flow fractions from $a=0.50$ to $a=0.005$. These values of TaRRs < 1 are characteristic for the active ventilation model, which by the very nature of the model will always produce such values. (The TaRR results for this SX-103 active ventilation case are shown in subsection 7.1 of the Appendix.)

As mentioned above, the results for the three cases presented in this section were representative of the range of results obtained from a total set of nine cases. For a perspective on the time-at-risk values for SX-103 shown here, note that the headspace times at risk calculated by the AT-RESOLVE code for all 1000 instances of passive ventilation ranged from $1.0\text{E}+06$ to $2.0\text{E}+07$ seconds for TX-102, from $0.5\text{E}+06$ to $1.2\text{E}+06$ seconds for SX-103, and from $1.0\text{E}+06$ to $4.5\text{E}+07$ for TX-112. The significantly shorter times-at-risk for SX-103 is indicative of its significantly higher ventilation rate (see Table 2).

5.0 CONCLUSIONS

This report covered the construction and evaluation of a dynamic two-volume model that was used to relate ex-tank flammable gas concentrations to headspace concentrations for passively and actively vented single-shell tanks. The main purpose of the model was to provide quantitative results to help determine frequencies of potentially hazardous flammable gas conditions within ex-tank volumes. To attain this objective, the two-volume model was evaluated for a range of realistic input parameters. The resulting time-dependent headspace and ex-tank flammable gas concentrations were used to obtain corresponding headspace and ex-tank "times at risk." This quantity is defined as the total elapsed time for which the flammable gas concentration exceeded LFL_u . The main results of this study are given as time-at-risk ratios or "TaRRs," which are formed by dividing ex-tank times at risk by headspace times at risk, and are shown as a function of GRE volume. The main findings of this analysis are listed below, and their validity is, of course, subject to the validity of the model assumptions.

- Headspace concentrations that exceed LFL_u can cause ex-tank concentrations also to exceed LFL_u . The extent to which this occurs depends upon the ex-tank volume and assumed fraction of headspace gas exiting through ex-tank volume. For ex-tank flow fractions greater than about 20%, hazardous conditions within the ex-tank volume occurred as frequently as within the headspace (with ex-tank flammable gas concentrations closely tracking headspace concentrations). Although less frequently (for released gas greater than about 300 m³), smaller flow fractions gave rise to greater potentially hazardous conditions.
- For the parameters used in this study, the GRE duration was at least two orders-of-magnitude smaller than the headspace or ex-tank times at risk – even for the active ventilation cases.
- For the parameters used in this study, all values of times at risk were found to be much larger than the (3.6E+03 seconds) mixing time required for the headspace to reach homogeneity. This is consistent with the "well-mixed" base assumption of the model.

Recommendations for Further Consideration

As mentioned above, the GRE threshold value of about 300 m³ was seen to produce ex-tank hazardous conditions that exceeded those within the headspace. These results were, for the most part, independent of flow fraction (parameter "a") and tank geometry. The underlying cause for such behavior appears to be the ability of the passive ventilation to eventually catch up to the GRE. This seems logical, but has not been extensively tested either by numerical sensitivity studies or experimentally. Until further confirmation of such a threshold, the apparent universality of this value suggests a possible limitation to the use of time-at-risk ratios.

6.0 REFERENCES

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7.0 APPENDIX

7.1 TIME-AT-RISK RATIOS (TaRRs) FOR VARIOUS EX-TANK VOLUMES

Figure 9: TaRR vs. GRE Vol. For TX-102, Sluice Pit

Figure 10: TaRR vs. GRE Vol. For TX-102, Pump Pit

Figure 11: TaRR vs. GRE Vol. For SX-103, Pump Pit **Figure 12: TaRR vs. GRE Vol. For SX-103, Condenser Hatchway**

Figure 13: TaRR vs. GRE Vol. For TX-112, Pump Pit-12A

Figure 14: TaRR vs. GRE Vol. For TX-112, Pump Pit-12B

Figure 15: TaRR vs. GRE Vol. For SX-103 (ACTIVE VENT), Pump Pit **Figure 16: TaRR vs. GRE Vol. For SX-103 (ACTIVE VENT.), Condenser Hatchway**

7.2 EX-TANK DATA

Representative Ex-tank Volumes

TX-112 (H-2-73130 Titled: Piping Waste Tank Isolation 241-TX-112)

(H-2-73634 6/11 tabulates these TX-112 ex-tank volumes, references)

Pump Pit 12A (H-2-35221) $5'9" \times (7'2" + 2'0") \times 4'6" \Rightarrow 6.7164 \text{ m}^3$
 Heat Exchanger Pit C (H-2-36637) $7'0" \times 12'0" \times 8.18" \Rightarrow 19.4571 \text{ m}^3$
 Valve Pit 1 (H-2-36638) isolated, backfilled per H-2-73130
 Valve Pit 2 (H-2-36638) isolated, backfilled per H-2-73130
 Instrument Pit (H-2-36638) isolated, backfilled per H-2-73130
 Pump Pit 12B (H-2-36636) $8'0" \times 9'10" \times 19'32" \times 7'6" \Rightarrow 16.7910 \text{ m}^3$
 Liquid Level Well Pit (H-2-73050) isolated, backfilled per H-2-73130
 Steam Trap Pit (H-2-35203) isolated, backfilled per H-2-73130
 Flow Meter Pit (H-2-73050) isolated, backfilled per H-2-73130

SX-103 (H-2-73220 Titled: Piping Waste Tank Isolation 241-SX-103)

(H-2-73634 10/11 tabulates these SX-103 ex-tank volumes, references)

Pump Pit 241-SX-03B (H-2-46150) $12'3" \times 7'0" \times 4'9" \Rightarrow 11.5338 \text{ m}^3$
 Pump Pit 241-SX-03A (H-2-3403) $5'0" \times 6'6" \times 6'0" \Rightarrow 5.5218 \text{ m}^3$
 Hatchway (H-2-39514) $5'9" \times 3'3" \times 12'3" \Rightarrow 6.4823 \text{ m}^3$
 Weight Factor Enclosure (H-2-70609) not connected to tank headspace

TX-102 (H-2-73118 Titled: Piping Waste Tank Isolation 241-TX-102)

(H-2-73634 6/11 tabulates TX-102 ex-tank volumes, references)

Cascade Sluice Pit 02C (H-2-42066) $10'10" \times 9'0" \times 6'5" \times 1'8" \Rightarrow 17.7445 \text{ m}^3$
 Cascade Sluice Pit 02D (H-2-42066) $10'10" \times 9'0" \times 6'5" \times 1'8" \Rightarrow 17.7445 \text{ m}^3$
 Cascade Pump Pit 02A (H-2-42065) $14'6" \times 11'0" \times 5'5" \times 3'4" \Rightarrow 24.7469 \text{ m}^3$
 Hatchway (H-2-816*) $5'9" \times 3'3" \times 12'3" \Rightarrow 6.4823 \text{ m}^3$
 Weight Factor Enclosure (H-2-70844-2) eliminated per H-2-73451 detail 5
 Liquid Level Well Pit (H-2-73050) isolated, backfilled per H-2-73118
 Flush Pit (H-2-35875-1) isolated, backfilled per H-2-73118

*H-2-816 is void, H-2-39514 seems to have same information, and was used.

Representative Ex-tank Flow Fractions

TX-112 (H-2-73130 Titled: Piping Waste Tank Isolation 241-TX-112)

Pump Pit 12A 4" Drain (R2)
 Pump Pit 12B 6" Drain (R9) to 42" Riser (R9)
 Heat Exchanger Pit 12C 6" Drain (R11) to 42" Riser (R11)
 To Atmosphere 4" Port with air filter (R10A)

Impression: $\approx 1/2$ to $\approx 3/4$ of passive ventilation flow could be through pump pits 12A or 12B or heat exchanger pit 12D.

SX-103 (H-2-73220 Titled: Piping Waste Tank Isolation 241-SX-103)

Pump Pit SX-03A 4" Drain (R1), 12" Riser (R5)
 Pump Pit SX-03B 4" Drain (R4), 12" Risers (R8 & R9)
 Condenser Hatchway 24" Conduit

To Atmosphere 4" Riser with air filter (R16)

Impressions: $\approx 1/2$ of passive ventilation flow could be through pump pits 03A or 03B with full flow through the condenser hatchway. Direction of natural circulation flow is expected to be from the atmosphere in through the condenser hatchway and from the tank headspace out through the pump pits 03A and 03B because the hatchway conduit is at the side of the tank dome and the entrance extends into the head space, while the risers to the pump pits are located closer to the center of the dome, and are at a higher elevation.

TX-102 (H-2-73118 Titled: Piping Waste Tank Isolation 241-TX-102)

Pump Pit 02A	4" Drain (R2)
	3" Drains (R5 & R14),
	12" Risers (R6 & R7),
	12" Air Lift Circulator (R13B)
Sluice Pit 02C	14" Air Lift Circulator (R10B)
Sluice Pit 02D	14" Air Lift Circulator (R12B)
Condenser Hatchway	24" Conduit
To Atmosphere	4" Line to air filter (R9A)

Impression: All of passive ventilation flow could be through pump pit 02A and through the condenser hatchway.

Direction of natural circulation flow is expected to be from the atmosphere in through the condenser hatchway and from the tank headspace out through the pump pit 02A because the hatchway conduit is at the side of the tank dome and the entrance extends into the head space, while the risers to the pump pit are located closer to the center of the dome, and are at a higher elevation.

The impression that most of the passive ventilation flow exits through some ex-tank volume is consistent with the results listed in Table 6.2 of the recent Organic Solvent Topical by Cowley 1997.

7.3 FORTRAN CODE EXTANK

The computer code EXTANK, written in the FORTRAN/77 programming language, was used to compute the times at risk in the ex-tank volume from headspace flammable gas concentration input data files. These input data files were written as output text files by a special debug Version 1.42 of the AT-RESOLVE code. This version was written by Steve Humphreys, and creates a text output file that contains specific AT-RESOLVE data relating to flammable gas concentrations. The EXTANK code consists of 10 separate program units (main program, 5 subroutines, and 4 functions). These program divisions are described separately:

Main Program. This program division: 1) reads the AT-RESOLVE generated text file, 2) establishes V_2 , the ex-tank volume, 3) establishes "a", the ex-tank volume ventilation flow fraction, 4) calls the ODE1, and ODE3 program subroutines, and 5) outputs the final FORTRAN unit 2 output. Optionally, AT-RESOLVE text file input can be written as output to FORTRAN unit 10. Debug information regarding calculations in process can be written as output to FORTRAN unit 11.

Subroutine ODE1. This subroutine does ex-tank volume flammable gas concentration calculations for the well-mixed headspace, passive ventilation, natural circulation assumption. This program division: 1) calculates the maximum flammable gas concentration in the headspace and in the ex-tank volume, 2) calculates the LFL_u time at risk for the tank headspace and the ex-tank volume, 3) accesses function DY2DT1 and function Y21.

Function DY2DT1. This function calculates the derivative of the flammable gas molar fraction in the ex-tank volume. The case is for the well-mixed headspace, passive ventilation, and natural circulation assumption. This function is used to determine the time of the maximum flammable gas concentration in the ex-tank volume.

Function Y21. This function calculates the flammable gas molar fraction in the ex-tank volume. The case is the well-mixed headspace, passive ventilation, and natural circulation assumption. This function is used to determine the time at risk for the ex-tank volume.

Subroutine ODE3. This subroutine does ex-tank volume flammable gas concentration calculations for the active ventilation, well-mixed headspace, natural circulation assumption. This program division: 1) calculates the maximum flammable gas concentration in the headspace and in the ex-tank volume, 2) calculates the LFL_u time at risk for the tank headspace and the ex-tank volume, 3) accesses function Y13 and function Y23.

Function Y13. This function calculates the flammable gas molar fraction in the tank headspace. The case is the active ventilation, well-mixed headspace, and natural circulation assumption. This function is used to determine the time at risk for the tank headspace.

Function Y23. This function calculates the flammable gas molar fraction in the ex-tank volume. The case is the active ventilation, well-mixed headspace, and natural circulation assumption. This function is used to determine the time at risk for the ex-tank volume.

The following comments are included to indicate the actual file names and other details related to the actual calculations performed with EXTANK.

For the passive ventilation cases, the AT-RESOLVE input files were obtained from the publicly accessible directories on the Hanford Local Area Network (HLAN) server \\APO12:

```
\\APO12\RESOLVE\Board\data\sx-103\sx103nc1.afi
\\APO12\RESOLVE\Braun\data\tx112nc1.afi
\\APO12\RESOLVE\Webb\tx102nc1.afi
```

These files were used as input for the special debug Version 1.42 of the AT-RESOLVE, and the cases were run by Dave Braun on 3 March 1998. The text output files were placed in:

```
\\APO12\RESOLVE\Witek~1\data\sx103n~1.txt
\\APO12\RESOLVE\Witek~1\data\tx102n~1.txt
\\APO12\RESOLVE\Witek~1\data\tx112n~1.txt
```

These AT-RESOLVE text output files were read as EXTANK input, which wrote its output to FORTRAN unit 2. The EXTANK code was used compute results for all three representative tanks considered in the passive ventilation case, each tank having three different ex-tank volumes, and each ex-tank volume evaluated with three different values of flow fractions.

For the active ventilation case, the EXTANK code was used to evaluate one tank (SX-103) for three different ex-tank volumes, and again with three different flow fractions for each volume. The file names on the tps3 computer on the SECC system were titled:

```
/tmp_mnt/home/h54413/fg/f02sx103_*.dat (18 cases),
/tmp_mnt/home/h54413/fg/f02tx102_*.dat (9 cases), an
/tmp_mnt/home/h54413/fg/f02tx112_*.dat (9 cases).
```

* _ represents a unique and distinguishing letter.

The EXTANK unit 2 output files for these different cases was used as input for the spreadsheet program, producing the results presented in this report. For completeness, a listing the EXTANK code is given next, and at the end of the code are partial listings of example input and output data. The partial listing of the AT-RESOLVE output/ EXTANK input for simulation instance 375, and the partial output (EXTANK to unit 2) is for a few instances, including 375.

```

c program extank by Warren D. Wittekind, FDNW (509)376-8175
c and Robert Ruben, FDNW (509)372-1995
c for a representative ex-tank region
c inputs data for headspace hydrogen concentration
c inputs data for frequencies of GRE occurrence
c calculates maximum hydrogen concentration
c calculates over-pressure of well-mixed burn
c outputs frequencies, over-pressure
c
c RESOLVE-AT output special debug (ver. 1.42) file values
c icase is the integer sequence number
c vambnt is Volume of Tank Headspace (meters**3)
c pambnt is Pressure of Tank Headspace (Pascals)
c tambnt is Temperature of Tank Headspace (deg K)
c volvnt is Ventilation rate Tank (meters**3/s)
c
c x(9) is initial headspace gas composition (moles)
c xt is initial headspace total gas content (moles)
c
c xg(3,9) is GRE (sml,med,large) gas composition (moles)
c xg(3) is GRE (sml,med,large) total gas content (moles)
c trel(3) is GRE release time for xg(3,9) composition (seconds)
c grat(3) is GRE (sml,med,large) gas release rate (meters**3/s)
c
c xgs(3,9) is Layer (sml,med,large) gas composition (moles)
c xgts(3) is Layer (sml,med,large) total gas content (moles)
c
c trisk(1,3) is layer gas time at risk (H2 > LFLu) (seconds)
c trisk(2,3) is mixed gas time at risk (H2 > LFLu) (seconds)
c freq(4,3) is frequency of such GREs for 4 activities (per year)
c
c CALCULATIONAL VALUES
c vhead is the total headspace volume (meters**3)
c rsg is GRE source term (meters**3/second)
c rvent is ventilation rate (meters**3/second)
c aa is fraction of rvent through ex-tank (dimensionless)
c v2 is ex-tank volume (meters**3)
c
c CALCULATED VALUES
c xlfu is lower flammability limit - upward (mole fraction)
c xlfd is lower flammability limit - downward (mole fraction)
c y1max is peak H2 headspace concentration (mole fraction)
c y2max is peak H2 ex-tank concentration (mole fraction)
c t1ursk is headspace time at risk - upward (seconds)
c t1drsk is headspace time at risk - downward (seconds)
c t2ursk is ex-tank time at risk - upward (seconds)
c t2drsk is ex-tank time at risk - downward (seconds)
c pres is delta pressure from burn (psi)
c cpburn is specific heat for combusted gas (Joules/kilogram-K)
c dose is radiological exposure (Sieverts)
c
c real*8 dat, xg1(9), xg2(9), xg3(9), xc(3,9), xct(3)
c real*8 vamb, pamb, tamb, vvrt, mvrt, xc1(9), xc2(9), xc3(9)
c real x(9), xt, xg(3,9), xgt(3), freq(4,3), trel(3), vm(3)
c real trisk(2,3)
c integer cntrdat, i, icase
c logical flam(3)
c character cntr*8, var1*11, var2*11
c character eqq, nothing*11, dum2(4)*5, dum1*5
c character test*11, test2*11, test3*11, test4*11, test20*11
c character test30*11, test40*11
c character cntr*8, var1*11, var2*11
c common / calcd / xlfu, xlfd, y1max, t1ursk, t1drsk,
c & y2max, t2ursk, t2drsk, pres, cpburn, dose
c common / inpt / icase, pambnt, x(9), xt, xg(3,9), xgt(3),
c & trel(3), grat(3), xgs(3,9), xgts(3),
c & trisk(2,3), freq(4,3)
c common /ypdat/ vhead, rsg, rvent, v2, aa, reff

```

```

c
open(unit = 1, file = 'sx103nc1.txt', status = 'old')
open(unit = 2, file = 'f02s103j.dat', status = 'unknown')
open(unit=10, file = 'f10s103j.dat', status = 'unknown')
open(unit=11, file = 'f11s103j.dat', status = 'unknown')
c
v2=6.4823
aa=0.200
c
*****
c
Write Output Data to unit 2
c
*****
write (2,900)
900 format (1x,'icase GRE',11x,'rsg',8x,'trsl',6x,'y1 max',5x,
& 't1urisk',5x,'t1drisk',6x,'y2 max',5x,'t2urisk',5x,'t2drisk')
c
*****
c
Read Input Data From RESOLVE-AT Output-Special Debug Version
c
*****
do 4 i = 1,3
  read (1,3)
3 format (a)
4 continue
5 read (1,3)
  read (1,*) cntr, eqq, cntrdat
  if (cntr .eq. "thisInst") i = cntrdat
  read (1,*) var1, eqq, vamb
  read (1,*) var1, eqq, pamb
  read (1,*) var1, eqq, tamb
  read (1,3)
  read (1,*) var1, eqq, vvrtr
  read (1,*) var1, eqq, mvrt
  read (1,3)
  read (1,*) cntr, eqq, cntrdat
  if (cntrdat .ne. i) print *, 'calcInitVariables', cntrdat, i
  if (cntrdat .ne. i) go to 5
  do 10 j = 1, 9
    x(j) = 0
10 continue
  test = " "
  j = 1
  do while (test .ne. "totalMolesA")
    read (1,*) var1, eqq, dat
    if (var1 .eq. "ammoniaMole") x(1) = dat
    if (var1 .eq. "argonMolesA") x(2) = dat
    if (var1 .eq. "carbonDioxi") x(3) = dat
    if (var1 .eq. "hydrogenMol") x(4) = dat
    if (var1 .eq. "methaneMole") x(5) = dat
    if (var1 .eq. "nitrogenMol") x(6) = dat
    if (var1 .eq. "nitrousOxid") x(7) = dat
    if (var1 .eq. "oxygenMoles") x(8) = dat
    if (var1 .eq. "waterVaporM") x(9) = dat
    if (var1 .eq. "totalMolesA") xt = dat
    test = var1
    j = j + 1
  end do
  read (1,3)
  read (1,*) cntr, eqq, cntrdat
  if (cntrdat .ne. i) print *, 'calcAmbientComposition', cntrdat, i
  if (cntrdat .ne. i) go to 5
  do 11 j = 1, 9
    xg1(j) = 0
11 continue
  j = 1
  test2 = " "
  do while (test2 .ne. "totalMolesG")
    read (1,*) var2, eqq, dat
    if (var2 .eq. "ammoniaMole") xg1(1) = dat

```

```

if (var2.eq. "argonMoloesA") xg1(2) = dat
if (var2.eq. "carbonDioxi") xg1(3) = dat
if (var2.eq. "methanMoloe") xg1(4) = dat
if (var2.eq. "nitrogenMoloe") xg1(5) = dat
if (var2.eq. "nitrogenMoloe") xg1(6) = dat
if (var2.eq. "nitrousOxid") xg1(7) = dat
if (var2.eq. "oxygMoloes") xg1(8) = dat
if (var2.eq. "waterVaporM") xg1(9) = dat
if (var2.eq. "totalMoloesG") xg1(1) = dat
test2 = = dat
! = ! + 1
end
do
read (1,*) nothing, eqq, var1(1)
read (1,*) nothing, eqq, var1(2)
do 12 ! = 1, 9
xg2(j) = 0
! = 1
test3 = = dat
do while (test3.eq. "totalMoloesG")
read (1,*) dat
if (var2.eq. "argonMoloesA") xg2(1) = dat
if (var2.eq. "carbonDioxi") xg2(2) = dat
if (var2.eq. "methanMoloesA") xg2(3) = dat
if (var2.eq. "nitrogenMoloe") xg2(4) = dat
if (var2.eq. "nitrogenMoloe") xg2(5) = dat
if (var2.eq. "nitrogenMoloe") xg2(6) = dat
if (var2.eq. "nitrousOxid") xg2(7) = dat
if (var2.eq. "oxygMoloes") xg2(8) = dat
if (var2.eq. "waterVaporM") xg2(9) = dat
if (var2.eq. "totalMoloesG") xg2(2) = dat
test3 = = dat
! = ! + 1
end
do 13 ! = 1, 9
read (1,*) nothing, eqq, var1(2)
read (1,*) nothing, eqq, var1(3)
xg3(j) = 0
! = 1
test4 = = dat
do while (test4.eq. "totalMoloesG")
read (1,*) dat
if (var2.eq. "argonMoloesA") xg3(1) = dat
if (var2.eq. "carbonDioxi") xg3(2) = dat
if (var2.eq. "methanMoloesA") xg3(3) = dat
if (var2.eq. "nitrogenMoloe") xg3(4) = dat
if (var2.eq. "nitrogenMoloe") xg3(5) = dat
if (var2.eq. "nitrogenMoloe") xg3(6) = dat
if (var2.eq. "nitrousOxid") xg3(7) = dat
if (var2.eq. "oxygMoloes") xg3(8) = dat
if (var2.eq. "waterVaporM") xg3(9) = dat
if (var2.eq. "totalMoloesG") xg3(3) = dat
test4 = = dat
! = ! + 1
end
do 26 k = 1, 9
read (1,*) nothing, eqq, var1(3)
read (1,*) nothing, eqq, var1(4)
xg(1,k) = xg1(k)
xg(2,k) = xg2(k)
xg(3,k) = xg3(k)
26 continue
read (1,*)
read (1,*) cnt, eqq, cntdat
if (cntdat.ne. i) print *, calcGrecComposition, cntdat, i
if (cntdat.ne. i) go to 5
do 27 j = 1, 9

```

```

    xc1(j) = 0
27 continue
    j = 1
    test20 = "      "
    do while (test20 .ne. "totalMolesL")
        read (1, *) var2, eqq, dat
        if (var2 .eq. "ammoniaMole") xc1(1) = dat
        if (var2 .eq. "argonMolesA") xc1(2) = dat
        if (var2 .eq. "carbonDioxi") xc1(3) = dat
        if (var2 .eq. "hydrogenMol") xc1(4) = dat
        if (var2 .eq. "methaneMole") xc1(5) = dat
        if (var2 .eq. "nitrogenMol") xc1(6) = dat
        if (var2 .eq. "nitrousOxid") xc1(7) = dat
        if (var2 .eq. "oxygenMoles") xc1(8) = dat
        if (var2 .eq. "waterVaporM") xc1(9) = dat
        if (var2 .eq. "totalMolesL") xc1(1) = dat
        test20 = var2
        j = j + 1
    end do
    read (1, *) nothing, eqq, flam(1)
    do 28 j = 1, 9
        xc2(j) = 0
28 continue
    j = 1
    test30 = "      "
    do while (test30 .ne. "totalMolesL")
        read (1, *) var2, eqq, dat
        if (var2 .eq. "ammoniaMole") xc2(1) = dat
        if (var2 .eq. "argonMolesA") xc2(2) = dat
        if (var2 .eq. "carbonDioxi") xc2(3) = dat
        if (var2 .eq. "hydrogenMol") xc2(4) = dat
        if (var2 .eq. "methaneMole") xc2(5) = dat
        if (var2 .eq. "nitrogenMol") xc2(6) = dat
        if (var2 .eq. "nitrousOxid") xc2(7) = dat
        if (var2 .eq. "oxygenMoles") xc2(8) = dat
        if (var2 .eq. "waterVaporM") xc2(9) = dat
        if (var2 .eq. "totalMolesL") xc2(1) = dat
        test30 = var2
        j = j + 1
    end do
    read (1, *) nothing, eqq, flam(2)
    do 30 j = 1, 9
        xc3(j) = 0
30 continue
    j = 1
    test40 = "      "
    do while (test40 .ne. "totalMolesL")
        read (1, *) var2, eqq, dat
        if (var2 .eq. "ammoniaMole") xc3(1) = dat
        if (var2 .eq. "argonMolesA") xc3(2) = dat
        if (var2 .eq. "carbonDioxi") xc3(3) = dat
        if (var2 .eq. "hydrogenMol") xc3(4) = dat
        if (var2 .eq. "methaneMole") xc3(5) = dat
        if (var2 .eq. "nitrogenMol") xc3(6) = dat
        if (var2 .eq. "nitrousOxid") xc3(7) = dat
        if (var2 .eq. "oxygenMoles") xc3(8) = dat
        if (var2 .eq. "waterVaporM") xc3(9) = dat
        if (var2 .eq. "totalMolesG") xc3(3) = dat
        test40 = var2
        j = j + 1
    end do
    read (1, *) nothing, eqq, flam(3)
    do 35 k = 1, 9
        xc(1,k) = xc1(k)
        xc(2,k) = xc2(k)
        xc(3,k) = xc3(k)
35 continue
    read (1, 3)

```

```

      read (1, *) cntr, eqq, cntrdat
      if (cntrdat .ne. i) print *, 'calcLayerComposition', cntrdat, i
      if (cntrdat .ne. i) go to 5
c   Stratified Layer - time at risk (small, med, large GREs)
      do 40 j = 1, 3
         read (1, *) nothing, eqq, trisk(1,j)
40  continue
      read (1, 3)
      read (1, *) cntr, eqq, cntrdat
      if (cntrdat .ne. i) print *, 'calcLayerTime', cntrdat, i
      if (cntrdat .ne. i) go to 5
c   Mixed Composition - time at risk (small, med, large GREs)
      do 50 j = 1, 3
         read (1, *) nothing, eqq, trisk(2,j)
50  continue
      do 70 j = 1, 4
         read (1, *) dum1, dum2(j)
         read (1, *) cntr, eqq, cntrdat
         if (cntrdat .ne. i) print *, 'calcMixedTime', cntrdat, i, j=' ', j
         if (cntrdat .ne. i) go to 5
         do 60 k = 1, 3
            read (1, *) nothing, eqq, freq(j,k)
60  continue
70  continue
c
c   *****
c   Convert Input Data From Double Precision to Single Precision
c   *****
      vambnt=vamb
      pambnt=pamb
      tambnt=tamb
      volvnt=vvrt
c   SX-103 is actively ventilated at 50 cfm, per pedigree database
      volvnt=50.0*4.7194744e-4
      do 75 k = 1, 3
         grat(k)=vrr(k)
         xgts(k)=xct(k)
         do 74 j=1,9
            xgs(k,j)=xc(k,j)
74  continue
75  continue
c
c   *****
c   Write Input Data From RESOLVE-AT Output-Special Debug Version
c   *****
c   write (10,100) i
c 100 format (/,'thisInstance =',15x,i5)
c   Tank Headspace Volume
c   write (10,101) vambnt
c 101 format (1x,'Tank Headspace Volume= ',f15.6,' meters**3')
c   Tank Headspace Pressure
c   write (10,102) pambnt
c 102 format (1x,'Tank Headspace Pressure =',f15.6,' Pascals')
c   Tank Headspace Temperature
c   write (10,103) tambnt
c 103 format (1x,'Tank Temperature= ',f15.6,' K')
c   Tank ventilation rate
c   write (10,104) volvnt
c 104 format (1x,'Ventilation Rate= ',1pe15.4,' m**3/s')
c   Headspace ambient composition
c   write (10,105) (x(k),k=1,9), xt
c 105 format (1x,'Ambient',10F12.4,' 0')
c   GRE composition - small GRE
c   write (10,106) (xg(1,k),k=1,9), xgt(1), trel(1), grat(1)
c 106 format (1x,'GRE dat',10F10.4,2(1pe10.2),' 1')
c   GRE composition - medium GRE
c   write (10,107) (xg(2,k),k=1,9), xgt(2), trel(2), grat(2)
c 107 format (1x,'GRE dat',10F10.4,2(1pe10.2),' 2')

```

```

c GRE composition - large GRE
c write (10,108) (xg(3,k),k=1,9), xgt(3), trl(3), grat(3)
c 108 format (1x,'GRE dat',10F10.4,2(1p10.2), '3')
c Layer composition - small GRE
c write (10,109) (xgs(1,k),k=1,9), xgts(1)
c 109 format (1x,'Layer s',10F12.4, '1')
c Layer composition - medium GRE
c write (10,110) (xgs(2,k),k=1,9), xgts(2)
c 110 format (1x,'Layer m',10F12.4, '2')
c Layer composition - large GRE
c write (10,111) (xgs(3,k),k=1,9), xgts(3)
c 111 format (1x,'Layer l',10F12.4, '3')
c Time At Risk, Stratified Layer, then Mixed Headspace
c write (10,112) (trisk(1,k),k=1,3)
c 112 format (1x,'TimeRisk',3(1p15.4), 'small, med, large')
c write (10,112) (trisk(2,k),k=1,3)
c Frequency of Spontaneous GRE's (per year)
c write (10,113) (freq(1,k),k=1,3)
c 113 format (1x,'Spontane',3(1p15.4), 'small, med, large')
c Frequency of Locally Waste Disturbing GRE's (per year)
c write (10,114) (freq(2,k),k=1,3)
c 114 format (1x,'LocalWas',3(1p15.4), 'small, med, large')
c Frequency of Globally Waste Disturbing GRE's (per year)
c write (10,115) (freq(3,k),k=1,3)
c 115 format (1x,'GlobalWa',3(1p15.4), 'small, med, large')
c Frequency of Seismically Induced GRE's (per year)
c write (10,116) (freq(4,k),k=1,3)
c 116 format (1x,'SeismicI',3(1p15.4), 'small, med, large')
c
c if (i.eq.(250*int(j/250))) write (2,900)
c
c *****
c Calculate Data For Ex-Tank reion from RESOLVE-AT Debug Version
c *****
icase=i
do 80 k=1,3
c vhead=Tank Headspace Volume (meters**3)
vhead=vambnt
c
c rsg=GRE Volume Flow Rate (meters**3/s)
rsg=grat(k)
c
c rsg=Tank Ventilation Flow Rate (meters**3/s)
rvent=volvnt
c
c v2=Ex-Tank=Saltwell Riser=HNF-SD-WM-SARR-036 p.6-17 (meters**3)
c 6 m x Pi/4 x (0.0254 x 10.020)**2 = 0.305242 m**3
c v2=Ex-Tank=Pump Pit=WHC-SD-WM-ER-571 p.21 (meters**3)
c 14 ft x 4.5 ft x 8 ft x (.3048)3 = 14.2717 meters**3
c v2=14.2717
c
c aa=Ex-Tank Flow fractionHNF-SD-WM-SARR-036 p.6-21 (dimensionless)
c 10.17 m**3/s / 13.88 m**3/s = 0.732709
c aa=0.732709
c
c Mixed Headspace composition cases, med & large GREs only
c if (k.gt.1.and.trisk(2,k).gt.0.0) then
c write (11,300) icase, k, trisk(2,k)
c 300 format (1x,'DEBUG',5x,'Before ODE1 call',5x,2i5,1p15.4)
c call odel(k)
c write (11,301) icase, k, y1max, y2max
c 301 format (1x,'DEBUG',5x,'After ODE1 call',5x,2i5,2(1p15.4))
c call calcon(k)
c write (2,901) icase, k, xgt(k), y1max, t1ursk, t1drsk,
& y2max, t2ursk, t2drsk
c &
c endif
c
c Mixed Headspace composition cases, med & large GREs only

```



```

if (k.gt.1.and.trisk(2,k).gt.0.0) then
c   write (11,400) icase, k, trisk(2,k)
c 400 format (1x,'DEBUG',5x,'Before ODE3 call',5x,2i5,1pe15.4)
      call ode3 (k)
c   write (11,401) icase, k, y1max, y2max
c 401 format (1x,'DEBUG',5x,'After ODE3 call ',5x,2i5,2(1pe15.4))
      write (2,901) icase, k, vrn(k), trel(k),
&      y1max, t1ursk, t1drsk, y2max, t2ursk, t2drsk
901 format (1x,2i5,1pe15.5,0pf12.3,2(0pf12.6,1pe12.4,1pe12.4))
      endif
80 continue
c
c   if (icase.gt.100) stop
c   if (icase.le.1000) go to 5
c
c   end
c   subroutine ode1 (k)
c   PASSIVE VENTILATION - NATURAL CIRCULATION
c   Accepts GRE Molar Composition, and time of release
c   Calculates Ex-Tank Region maximum flammable gas concentration, and
c   Calculates Ex-Tank Region time at Risk (upward-lfl & downward-lfl)
c
c   common / calcd / xlfu, xlfld, y1max, t1ursk, t1drsk,
&   y2max, t2ursk, t2drsk, pres, cpburn, dose
c   common / inpt / icase, pambnt, x(9), xt, xg(3,9), xgt(3),
&   trel(3), grat(3), xgs(3,9), xgts(3),
&   trisk(2,3), freq(4,3)
c   common /ypdat/ vhead, rsg, rvent, v2, aa, reff
c   dimension tflfd(5), tflfu(5)
c
c   Lower flammability limits (molar fraction) for NH3, H2, & CH4.
c   From RESOLVE (constan0.f90 page 10 of 11) dated 17 Dec 1997.
c   data tflfd(1), tflfd(4), tflfd(5) / 0.18, 0.08, 0.063 /
c   data tflfu(1), tflfu(4), tflfu(5) / 0.15, 0.04, 0.05 /
c
c   R, the universal gas constant (Pa m3 / mol K) or (J / mol K)
c   From RESOLVE (constan0.f90 page 8 of 11) dated 17 Dec 1997.
c   data r / 8.31441 /
c
c   MIXED HEADSPACE COMPOSITION APPLICATION
c   returns the maximum flammable gas concentration
c   calculates the flammable gas time at risk - upward & downward
c   x(9) is initial headspace gas composition (moles)
c   xt is initial headspace total gas content (moles)
c   xg(3,9) is GRE (sml,med,large) mixed gas composition (moles)
c   xgt(3) is GRE (sml,med,large) mixed total gas content (moles)
c   trel(3) is GRE release time for xg(3,9) composition (seconds)
c   trisk(1,3) is layer gas time at risk (H2 > LFLu) (seconds)
c   trisk(2,3) is mixed gas time at risk (H2 > LFLu) (seconds)
c   freq(4,3) is frequency of such GREs for 4 activities (per year)
c
c   CALCULATIONAL VALUES
c   vhead is the total headspace volume (meters**3)
c   rsg is GRE source term (meters**3/second)
c   rvent is ventilation rate (meters**3/second)
c   rsg=grat(k)
c
c   CALCULATED VALUES
c   xlfu is lower flammability limit - upward (mole fraction)
c   xlfld is lower flammability limit - downward (mole fraction)
c   y1max is peak H2 headspace concentration (mole fraction)
c   y2max is peak H2 ex-tank concentration (mole fraction)
c   t1ursk is headspace time at risk - upward (seconds)
c   t1drsk is headspace time at risk - downward (seconds)
c   t2ursk is ex-tank time at risk - upward (seconds)
c   t2drsk is ex-tank time at risk - downward (seconds)
c   pres is delta pressure from burn (psi)
c   cpburn is specific heat for combusted gas (Joules/kilogram-K)

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c   dose is radiological exposure           (Sieverts)
c
c   initial calculations for hydrogen gas flammability (LFLu & LFLd)
xflfu=1.0/((xg(k,1)*xg(k,4))/tflfu(1)+1./tflfu(4)
& +(xg(k,5)*xg(k,4))/tflfu(5))
xflfd=1.0/((xg(k,1)*xg(k,4))/tflfd(1)+1./tflfd(4)
& +(xg(k,5)*xg(k,4))/tflfd(5))
c
c   calculations for time at risk in tank headspace
y0=xg(k,4)*xgt(k)
reff=max(rsg,rvent)
y1max=(y0*rsg/reff)*(1.0-exp(-trel(k)*reff/vhead))
t1ursk=0.0
t1drsk=0.0
if (y1max.ge.xflfu) then
  tu1=-(vhead/reff)*log(1.0-xflfu*(reff/(y0*rsg)))
  tu2=trel(k)-(vhead/rvent)*log(xflfu/y1max)
  t1ursk=tu2-tu1
endif
if (y1max.ge.xflfd) then
  td1=-(vhead/reff)*log(1.0-xflfd*(reff/(y0*rsg)))
  td2=trel(k)-(vhead/rvent)*log(xflfd/y1max)
  t1drsk=td2-td1
endif
c
c   write (11,100) xflfu, y1max, tu1, tu2, t1ursk, k
c   write (11,100) xflfd, y1max, td1, td2, t1drsk, k
c 100 format (1x,DEBUG 1ODE1',5(1pe11.4),i5)
c
c   CALCULATIONS for TIME AT RISK in ex-tank region
c
c   maximum ex-tank flammable gas molar fraction
j=1
i=0
tlo=trel(k)
thi=trel(k)+trisk(2,k)
ftlo=dy2dt1(k,tlo)
fthi=dy2dt1(k,thi)
1 tnew=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
if ((thi-tnew)/thi.lt.1.e-2.and.i.le.10) tnew=0.1*(9.*tlo+thi)
ftnew=dy2dt1(k,tnew)
i=i+1
c   write (11,200) tnew, ftnew, tlo, ftlo, thi, fthi, i, j
c 200 format (1x,DEBUG 1ODE1',6(1pe11.4),2i5)
if (ftnew.lt.0.0) then
  thi=tnew
  fthi=ftnew
else
  tlo=tnew
  ftlo=ftnew
endif
if (abs(ftnew).gt.2.e-10.and.thi-tlo.gt.50.0) go to 1
t2max=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
y2max=y21(k,t2max)
t2ursk=0.0
t2drsk=0.0
ftmax=dy2dt1(k,t2max)
c   write (11,200) tnew, ftnew, t2max, ftmax, t2max, y2max, i, j
c
c   calculations for time at risk LFL-upward
if (y2max.ge.xflfu) then
c   calculations for start of time at risk LFL-upward
j=0
j=2
tlo=0.0
thi=t2max
ftlo=0.0-xflfu
fthi=y21(k,thi)-xflfu

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2  tnew=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
   if ((thi-tnew)/thi.lt.1.e-2.and.i.le.5) tnew=0.2*(4.*tlo+thi)
   ftnew=y21(k,tnew)-xflfu
   i=i+1
c   write (11,200) tnew, ftnew, tlo, ftlo, thi, fthi, i, j
   if (ftnew.gt.0.0) then
       thi=tnew
       fthi=ftnew
   else
       tlo=tnew
       ftlo=ftnew
   endif
   if (abs(ftnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 2
   tu1=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
   ftu1=y21(k,tu1)-xflfu
c   write (11,200) tu1, ftu1, tlo, ftlo, thi, fthi, i, j
c   calculations for end of time at risk LFL-upward
   i=0
   j=3
   tlo=t2max
   thi=t2max+trisk(2,k)
   ftlo=y21(k,tlo)-xflfu
   fthi=y21(k,thi)-xflfu
3  tnew=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
   if ((thi-tnew)/thi.lt.1.e-2.and.i.le.3) tnew=0.1*(9.*tlo+thi)
   ftnew=y21(k,tnew)-xflfu
   i=i+1
c   write (11,200) tnew, ftnew, tlo, ftlo, thi, fthi, i, j
   if (ftnew.lt.0.0) then
       thi=tnew
       fthi=ftnew
   else
       tlo=tnew
       ftlo=ftnew
   endif
   if (abs(ftnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 3
   tu2=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
   ftu2=y21(k,tu2)-xflfu
c   write (11,200) tu2, ftu2, tlo, ftlo, thi, fthi, i, j
   t2ursk=tu2-tu1
   endif
c
c   calculations for time at risk LFL-downward
   if (y2max.ge.xfld) then
c   calculations for start of time at risk LFL-downward
       j=4
       tlo=0.0
       thi=t2max
       ftlo=0.0-xfld
       fthi=y21(k,thi)-xfld
4  tnew=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
   if ((thi-tnew)/thi.lt.1.e-2.and.i.le.5) tnew=0.2*(4.*tlo+thi)
   ftnew=y21(k,tnew)-xfld
   i=i+1
c   write (11,200) tnew, ftnew, tlo, ftlo, thi, fthi, i, j
   if (ftnew.gt.0.0) then
       thi=tnew
       fthi=ftnew
   else
       tlo=tnew
       ftlo=ftnew
   endif
   if (abs(ftnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 4
   td1=tlo-ftlo*(tlo-thi)/(ftlo-fthi)
c   calculations for end of time at risk LFL-downward
   j=5
   tlo=t2max
   thi=t2max+trisk(2,k)

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f1o=y21(k,t1o)-x1f1d
fthi=y21(k,thi)-x1f1d
5  tnew=t1o-f1o*(t1o-thi)/(f1o-fthi)
   if ((thi-tnew)/thi.lt.1.e-2.and.i.le.3) tnew=0.1*(9.*t1o+thi)
   f1new=y21(k,tnew)-x1f1d
   i=i+1
c   write (11,200) tnew, f1new, t1o, f1o, thi, fthi, i, j
   if (f1new.lt.0.0) then
       thi=tnew
       fthi=f1new
   else
       t1o=tnew
       f1o=f1new
   endif
   if (abs(f1new).gt.1.e-6.and.thi-t1o.gt.50.0) go to 5
   td2=t1o-f1o*(t1o-thi)/(f1o-fthi)
   t2drsk=td2-td1
endif

c
c   write (11,101) x1f1u, y2max, tu1, tu2, t2ursk, k
c   write (11,101) x1f1d, y2max, td1, td2, t2drsk, k
c 101 format (1x,DEBUG 2ODE1',5(1pe11.4),i5)
      return
      end
      function dy2dt1(k,t)
c  PASSIVE VENTILATION - NATURAL CIRCULATION
c  calculates derivative of ex-tank region flammable gas molar fraction
      common / inpt / icase, pambnt, x(9), xt, xg(3,9), xgt(3),
      &          trel(3), grat(3), xgs(3,9), xgts(3),
      &          trisk(2,3), freq(4,3)
      common /ypdat/ vhead, rsg, rvent, v2, aa, reff
      reff=max(rsg,rvent)
      y0=xg(k,4)/xgt(k)
      if (t.le.trel(k)) then
c 0 <= t <= tau-release
      dy2dt1=(y0*rsg*aa/(v2-aa*vhead))*
      & (exp(-t*aa*reff/v2)-exp(-t*reff/vhead))
      else
c tau-release <= t < infinity
      dy2dt1=(y0*rsg/reff)*(1.0-exp(-(trel(k)*reff/vhead)))*
      & ((aa*vhead/v2)/(1.0-aa*vhead/v2))*
      & ((rvent/vhead)*exp(-(t-trel(k))*rvent/vhead)-
      & (aa*rvent/v2)*exp(-(t-trel(k))*aa*rvent/v2))+
      & (y0*rsg/(reff-aa*reff*vhead/v2))*
      & (1.0-exp(-(trel(k)*aa*reff/v2)-
      & (aa*vhead/v2)*(1.0-exp(-(trel(k)*reff/vhead)))*
      & (-aa*rvent/v2)*exp(-(t-trel(k))*aa*rvent/v2)
      endif
      return
      end
      function y21(k,t)
c  PASSIVE VENTILATION - NATURAL CIRCULATION
c  calculates magnitude of ex-tank region flammable gas molar fraction
      common / inpt / icase, pambnt, x(9), xt, xg(3,9), xgt(3),
      &          trel(3), grat(3), xgs(3,9), xgts(3),
      &          trisk(2,3), freq(4,3)
      common /ypdat/ vhead, rsg, rvent, v2, aa, reff
      reff=max(rsg,rvent)
      y0=xg(k,4)/xgt(k)
      if (t.le.trel(k)) then
c 0 <= t <= tau-release
      y21=(y0*rsg/(reff-aa*reff*vhead/v2))*
      & ((1.0-exp(-(t*aa*reff/v2))-
      & (aa*vhead/v2)*(1.0-exp(-(t*reff/vhead))
      else
c tau-release <= t < infinity
      y21=(y0*rsg/reff)*(1.0-exp(-(trel(k)*reff/vhead)))*
      & ((aa*vhead/v2)/(1.0-aa*vhead/v2))*

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& (-exp(-(t-trel(k))*rvent/vhead)+
& exp(-(t-trel(k))*aa*rvent/v2))+
& (y0*rsq/(reff-aa*reff*vhead/v2))*
& (1.0-exp(-trel(k)*aa*reff/v2)-
& (aa*vhead/v2)*(1.0-exp(-trel(k)*reff/vhead))))*
& exp(-(t-trel(k))*aa*rvent/v2)
endif
return
end
subroutine ode3 (k)
c ACTIVE VENTILATION
c Accepts GRE Molar Composition, and time of release
c Calculates Ex-Tank Region maximum flammable gas concentration, and
c Calculates Ex-Tank Region time at Risk (upward-lfl & downward-lfl)
c
common / calcd / xlflu, xlflld, y1max, tlursk, tldrsk,
& y2max, t2ursk, t2drsk, pres, cpburn, dose
common / inpt / icase, pambnt, x(9), xt, xg(3,9), xgt(3),
& trel(3), grat(3), xgs(3,9), xgts(3),
& trisk(2,3), freq(4,3)
common /ypdat/ vhead, rsg, rvent, v2, aa, reff
dimension tlflld(5), tlflu(5)

c
c Lower flammability limits (molar fraction) for NH3, H2, & CH4.
c From RESOLVE (constan0.f90 page 10 of 11) dated 17 Dec 1997.
data tlflld(1), tlflld(4), tlflld(5) / 0.18, 0.08, 0.063 /
data tlflu(1), tlflu(4), tlflu(5) / 0.15, 0.04, 0.05 /

c
c R, the universal gas constant (Pa m3 / mol K) or (J / mol K)
c From RESOLVE (constan0.f90 page 8 of 11) dated 17 Dec 1997.
data r / 8.31441 /

c
c MIXED HEADSPACE COMPOSITION APPLICATION
c returns the maximum flammable gas concentration
c calculates the flammable gas time at risk - upward & downward
c X(9) is initial headspace gas composition (moles)
c xt is initial headspace total gas content (moles)
c xg(3,9) is GRE (sml,med,large) mixed gas composition (moles)
c xgt(3) is GRE (sml,med,large) mixed total gas content (moles)
c trel(3) is GRE release time for xg(3,9) composition (seconds)
c trisk(1,3) is layer gas time at risk (H2 > LFLu) (seconds)
c trisk(2,3) is mixed gas time at risk (H2 > LFLu) (seconds)
c freq(4,3) is frequency of such GREs for 4 activities (per year)
c
c CALCULATIONAL VALUES
c vhead is the total headspace volume (meters**3)
c rsg is GRE source term (meters**3/second)
c rvent is ventilation rate (meters**3/second)
c rsg=grat(k)

c
c CALCULATED VALUES
c xlflu is lower flammability limit - upward (mole fraction)
c xlflld is lower flammability limit - downward (mole fraction)
c y1max is peak H2 headspace concentration (mole fraction)
c y2max is peak H2 ex-tank concentration (mole fraction)
c tlursk is headspace time at risk - upward (seconds)
c tldrsk is headspace time at risk - downward (seconds)
c t2ursk is ex-tank time at risk - upward (seconds)
c t2drsk is ex-tank time at risk - downward (seconds)
c pres is delta pressure from burn (psi)
c cpburn is specific heat for combusted gas (Joules/kilogram-K)
c dose is radiological exposure (Sieverts)
c
c initial calculations for hydrogen gas flammability (LFLu & LFLd)
xlflu=1.0/((xg(k,1)*xg(k,4))/tlflu(1)+1./tlflu(4)
& +(xg(k,5)/xg(k,4))/tlflu(5))
xlflld=1.0/((xg(k,1)*xg(k,4))/tlflld(1)+1./tlflld(4)
& +(xg(k,5)/xg(k,4))/tlflld(5))

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c
c  calculations for time at risk in tank headspace
y0=xg(k,4)/xgt(k)
reff=max(rsg,rvent)
y1max=y0*(rsg/reff)*(1.0-exp(-trel(k)*reff/vhead))
t1ursk=0.0
t1drsk=0.0
if (y1max.ge.xlflu) then
  j=1
  i=0
  tu1=- (vhead/reff)*log(1.0-xlflu/y0)
c  calculations for end of time at risk LFL-upward
  tlo=trel(k)
  thi=trel(k)+trisk(2,k)
  flo=y13(k,tlo)-xlflu
  fthi=y13(k,thi)-xlflu
  if (fthi.gt.0.0) then
20   thi=thi*2.0
    fthi=y13(k,thi)
    if (fthi.gt.0.0) go to 20
  endif
  1  tnew=tlo-flo*(tlo-thi)/(flo-fthi)
    if (i.le.1) tnew=0.2*(4.*tlo+thi)
    fnew=y13(k,tnew)-xlflu
    i=i+1
c  write (11,200) tnew, fnew, tlo, flo, thi, fthi, i, j
c 200 format (1x,DEBUG ODE3',6(1pe11.4),2i5)
    if (fnew.lt.0.0) then
      thi=tnew
      fthi=fnew
    else
      tlo=tnew
      flo=fnew
    endif
    if (abs(fnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 1
    tu2=tlo-flo*(tlo-thi)/(flo-fthi)
    t1ursk=tu2-tu1
  endif
  if (y1max.ge.xlflld) then
    j=2
    i=0
    td1=- (vhead/rsg)*log(1.0-xlflld/y0)
c  calculations for end of time at risk LFL-downward
    tlo=trel(k)
    thi=trel(k)+trisk(2,k)
    flo=y13(k,tlo)-xlflld
    fthi=y13(k,thi)-xlflld
    if (fthi.gt.0.0) then
21   thi=thi*2.0
      fthi=y13(k,thi)
      if (fthi.gt.0.0) go to 21
    endif
    2  tnew=tlo-flo*(tlo-thi)/(flo-fthi)
      if (i.le.2) tnew=0.1*(9.*tlo+thi)
      fnew=y13(k,tnew)-xlflld
      i=i+1
c  write (11,200) tnew, fnew, tlo, flo, thi, fthi, i, j
c  if (fnew.lt.0.0) then
    thi=tnew
    fthi=fnew
  else
    tlo=tnew
    flo=fnew
  endif
  if (abs(fnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 2
  td2=tlo-flo*(tlo-thi)/(flo-fthi)
  t1drsk=td2-td1
endif

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c
c  write (11,100) xlf1u, y1max, tu1, tu2, t1ursk, k
c  write (11,100) xlf1d, y1max, td1, td2, t1drsk, k
c 100 format (1x,'DEBUG 1ODE3',5(1pe11.4),i5)
c
c  CALCULATIONS for TIME AT RISK in ex-tank region
c
  y2max=0.0
  t2ursk=0.0
  t2drsk=0.0
  if (rsg.le.rvent) go to 10
c
c  maximum ex-tank flammable gas molar fraction
  y2max=(y0/(1.0-aa*(rsg-rvent)*vhead/(rsg*v2)))*
  & (1.0-exp(-aa*(rsg-rvent)*trel(k)/v2))-
  & ((y0*aa*(rsg-rvent)/v2)/(rsg/vhead-aa*(rsg-rvent)/v2))*
  & (1.0-exp(-rsg*trel(k)/vhead))
c
c  calculations for time at risk LFL-upward
  if (y2max.ge.xlf1u) then
c  calculations for start of time at risk LFL-upward
    j=3
    i=0
    tlo=0.0
    thi=trel(k)
    f1lo=0.0-xlf1u
    f1hi=y23(k,thi)-xlf1u
  3  tnew=tlo-f1lo*(tlo-thi)/(f1lo-f1hi)
    f1new=y23(k,tnew)-xlf1u
    i=i+1
c  write (11,200) tnew, f1new, tlo, f1lo, thi, f1hi, i, j
    if (f1new.gt.0.0) then
      thi=tnew
      f1hi=f1new
    else
      tlo=tnew
      f1lo=f1new
    endif
    if (abs(f1new).gt.1.e-6.and.thi-tlo.gt.50.0) go to 3
    tu1=tlo-f1lo*(tlo-thi)/(f1lo-f1hi)
c  calculations for end of time at risk LFL-upward
    j=4
    i=0
    tlo=trel(k)
    thi=trel(k)+trisk(2,k)
    f1lo=y23(k,tlo)-xlf1u
    f1hi=y23(k,thi)-xlf1u
  4  tnew=tlo-f1lo*(tlo-thi)/(f1lo-f1hi)
    if (i.le.3) tnew=0.05*(19.0*tlo+thi)
    f1new=y23(k,tnew)-xlf1u
    i=i+1
c  write (11,200) tnew, f1new, tlo, f1lo, thi, f1hi, i, j
    if (f1new.lt.0.0) then
      thi=tnew
      f1hi=f1new
    else
      tlo=tnew
      f1lo=f1new
    endif
    if (abs(f1new).gt.1.e-6.and.thi-tlo.gt.50.0) go to 4
    tu2=tlo-f1lo*(tlo-thi)/(f1lo-f1hi)
    t2ursk=tu2-tu1
  endif
c
c  calculations for time at risk LFL-downward
  if (y2max.ge.xlf1d) then
c  calculations for start of time at risk LFL-downward
    j=5

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```

i=0
tlo=0.0
thi=trel(k)
fFlo=0.0-xlfld
fthi=y23(k,thi)-xlfld
5 tnew=tlo-flo*(tlo-thi)/(fFlo-fthi)
  fnew=y23(k,tnew)-xlfld
  i=i+1
c   write (11,200) tnew, fnew, tlo, fFlo, thi, fthi, i, j
   if (fnew.gt.0.0) then
     thi=tnew
     fthi=fnew
   else
     tlo=tnew
     fFlo=fnew
   endif
   if (abs(fnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 5
   td1=tlo-flo*(tlo-thi)/(fFlo-fthi)
c   calculations for end of time at risk LFL-downward
   j=6
   i=0
   tlo=trel(k)
   thi=trel(k)+trisk(2,k)
   fFlo=y23(k,tlo)-xlfld
   fthi=y23(k,thi)-xlfld
6  tnew=tlo-flo*(tlo-thi)/(fFlo-fthi)
   if (i.le.3) tnew=0.05*(19.0*tlo+thi)
   fnew=y23(k,tnew)-xlfld
   i=i+1
c   write (11,200) tnew, fnew, tlo, fFlo, thi, fthi, i, j
   if (fnew.lt.0.0) then
     thi=tnew
     fthi=fnew
   else
     tlo=tnew
     fFlo=fnew
   endif
   if (abs(fnew).gt.1.e-6.and.thi-tlo.gt.50.0) go to 6
   td2=tlo-flo*(tlo-thi)/(fFlo-fthi)
   t2drsk=td2-td1
   endif

c
c   write (11,101) xflu, y2max, tu1, tu2, tursk, k
c   write (11,101) xfld, y2max, td1, td2, t2drsk, k
c 101 format (1x,DEBUG 20DE3',5(1pe11.4),i5)
10 return
end
function y13(k,t)
c   ACTIVE VENTILATION
c   calculates magnitude of headspace flammable gas fraction
common / inpt / icaae, parmnt, x(9), xt, xg(3,9), xgt(3),
&      trel(3), grat(3), xgs(3,9), xgts(3),
&      trisk(2,3), freq(4,3)
common /ypdat/ vhead, rsg, rvent, v2, aa, reff
y0=xg(k,4)/xgt(k)
reff=max(rsg,rvent)
if (t.le.trel(k)) then
c   0 =< t =< tau-release
  y13=y0*(rsg/reff)*(1.0-exp(-t*reff/vhead))
else
c   tau-release =< t < infinity
  if (rsg.lt.reff) then
    y13=y0*(rsg/reff)*(1.0-exp(-trel(k)*reff/vhead))*
    & exp(-(t-trel(k))*rvent/vhead)
  else
    y13=y0*(1.0-exp(-trel(k)*rsg/vhead))*
    & exp(-(t-trel(k))*rvent/vhead)+
    & ((y0/(1.0-aa*(rsg-rvent))*vhead/(rsg*v2)))
  endif
endif

```



```

& (1.0-exp(-trel(k)*aa*(rsg-rvent)/v2))-
& ((y0*aa*(rsg-rvent)/v2)/(rsg/vhead-aa*(rsg-rvent)/v2))*
& (1.0-exp(-trel(k)*rsg/vhead)))*)
& ((aa/vhead)/(aa/v2-1.0/vhead))*
& (exp(-(t-trel(k))*rvent/vhead)-exp(-(t-trel(k))*aa*rvent/v2))
endif
endif
return
end
function y23(k,t)
c ACTIVE VENTILATION
c calculates magnitude of ex-tank region flammable gas molar fraction
common / inpt / icase, pambnt, x(9), xt, xg(3,9), xgt(3),
& trel(3), grat(3), xgs(3,9), xgts(3),
& trisk(2,3), freq(4,3)
common /ypdat/ vhead, rsg, rvent, v2, aa, reff
y0=xg(k,4)/xgt(k)
if (t.le.trel(k)) then
c 0 =< t =< tau-release
y23=(y0/(1.0-aa*(rsg-rvent)*vhead/(rsg*v2)))*
& (1.0-exp(-aa*(rsg-rvent)*t/v2))-
& ((y0*aa*(rsg-rvent)/v2)/(rsg/vhead-aa*(rsg-rvent)/v2))*
& (1.0-exp(-rsg*t/vhead))
else
c tau-release =< t < infinity
y23=((y0/(1.0-aa*(rsg-rvent)*vhead/(rsg*v2)))*
& (1.0-exp(-aa*(rsg-rvent)*trel(k)/v2))-
& ((y0*aa*(rsg-rvent)/v2)/(rsg/vhead-aa*(rsg-rvent)/v2))*
& (1.0-exp(-rsg*trel(k)/vhead)))*exp(-(t-trel(k))*aa*rvent/v2)
endif
return
end

```

=====

Debug Output File

Function afeMain:

afeFileSpecifier = C:\Program Files\Resolve\databases\SX103NC1

Function calcInitVariables:

```

thisInstance = 375
volumeAmbient = 2363.33194154000
pressureAmbient = 100914.251327900
temperatureAmbient = 301.849779833333
totalMolesAmbient = 95028.7304394498
volumetricVentilationRateTank = 0.471947440000000D-002
molarVentilationRateTank = 0.189768374340695

```

Function calcAmbientComposition:

```

thisInstance = 375
ammoniaMolesAmbient = 0.000000000000000
argonMolesAmbient = 883.767193086883
carbonDioxideMolesAmbient = 28.5086191318349
hydrogenMolesAmbient = 0.000000000000000
methaneMolesAmbient = 0.000000000000000
nitrogenMolesAmbient = 74207.9356001663
nitrousOxideMolesAmbient = 0.000000000000000
oxygenMolesAmbient = 19908.5190270647
waterVaporMolesAmbient = 0.000000000000000
totalMolesAmbient = 95028.7304394498

```

Function calcGreComposition:

```

thisInstance = 375
ammoniaMolesGre(greSmall) = 78.8430049759600
hydrogenMolesGre(greSmall) = 2463.84982572905
methaneMolesGre(greSmall) = 26.2707718059704
nitrogenMolesGre(greSmall) = 525.620011272233
nitrousOxideMolesGre(greSmall) = 190.541456668238
totalMolesGre(greSmall) = 3285.12507045145
wasteGreDuration(greSmall) = 87264.9000000000
volumetricRelRateGre(greSmall) = 0.107385191817220D-002
ammoniaMolesGre(greMedium) = 184.181398373498
hydrogenMolesGre(greMedium) = 5755.68252914058
methaneMolesGre(greMedium) = 61.3699019849640
NITROGENMOLESGRE(GREMEDIU) = 1227.87593799516
nitrousOxideMolesGre(greMedium) = 445.114844975531
totalMolesGre(greMedium) = 7674.22461246974
wasteGreDuration(greMedium) = 465.010000000000
volumetricRelRateGre(greMedium) = 0.470765141873593
ammoniaMolesGre(greLarge) = 1091.23096951841
HYDROGENMOLESGRE(GRELARGE) = 34101.0497367251
methaneMolesGre(greLarge) = 363.602069664479
nitrogenMolesGre(greLarge) = 7274.87282700301
nitrousOxideMolesGre(greLarge) = 2637.19956585786
totalMolesGre(greLarge) = 45467.9551687688
wasteGreDuration(greLarge) = 4254.16000000000
volumetricRelRateGre(greLarge) = 0.304876315562468

```

Function calcLayerComposition:

```

thisInstance = 375
ammoniaMolesLayer(greSmall) = 0.000000000000000
argonMolesLayer(greSmall) = 0.000000000000000
carbonDioxideMolesLayer(Small) = 0.000000000000000
hydrogenMolesLayer(greSmall) = 0.000000000000000
methaneMolesLayer(greSmall) = 0.000000000000000
nitrogenMolesLayer(greSmall) = 0.000000000000000
nitrousOxideMolesLayer(Small) = 0.000000000000000
oxygenMolesLayer(greSmall) = 0.000000000000000
waterVaporMolesLayer(greSmall) = 0.000000000000000
totalMolesLayer(greSmall) = 0.000000000000000
flammable(brnSmallLayer) = F
ammoniaMolesLayer(greMedium) = 184.181398373498
argonMolesLayer(greMedium) = 310.148209056917
carbonDioxideMolesLayer(Medium) = 10.0047809373199
hydrogenMolesLayer(greMedium) = 5755.68252914058

```

```

methaneMolesLayer(greMedium) = 61.3699019849640
nitrogenMolesLayer(greMedium) = 27270.3207178389
nitrousOxideMolesLayer(Medium) = 445.114844975531
oxygenMolesLayer(greMedium) = 6986.67202122840
waterVaporMolesLayer(greMedium) = 0.000000000000000
totalMolesLayer(greMedium) = 41023.4944035361
flammable(brnMediumLayer) = T
ammoniaMolesLayer(greLarge) = 0.000000000000000
argonMolesLayer(greLarge) = 0.000000000000000
carbonDioxideMolesLayer(Large) = 0.000000000000000
hydrogenMolesLayer(greLarge) = 0.000000000000000
methaneMolesLayer(greLarge) = 0.000000000000000
nitrogenMolesLayer(greLarge) = 0.000000000000000
nitrousOxideMolesLayer(Large) = 0.000000000000000
oxygenMolesLayer(greLarge) = 0.000000000000000
waterVaporMolesLayer(greLarge) = 0.000000000000000
totalMolesLayer(greLarge) = 0.000000000000000
flammable(brnLargeLayer) = T
Function calcLayerTime:
thisInstance = 375
timeRisk(brnSmallLayer) = 0.000000000000000
timeRisk(brnMediumLayer) = 4892.97993303125
timeRisk(brnLargeLayer) = 0.000000000000000
Function calcMixedTime:
thisInstance = 375
timeRisk(brnSmallMixed) = 0.000000000000000
timeRisk(brnMediumMixed) = 262090.109501572
timeRisk(brnLargeMixed) = 1048530.62996710
Function calcSpontaneousGre:
thisInstance = 375
spontaneousGre(greSmall) = 4.490270000000000
spontaneousGre(greMedium) = 0.314227000000000D-002
spontaneousGre(greLarge) = 0.692041000000000D-004
Function calcLocalGre:
thisInstance = 375
localGre(greSmall) = 0.455420728703000D-007
localGre(greMedium) = 0.764362487780000D-002
localGre(greLarge) = 0.455771710079000D-005
Function calcGlobalGre:
thisInstance = 375
globalGre(greSmall) = 0.408326665680000
GLOBALGRE(GREMEDIUM) = 0.115337239560000D-001
globalGre(greLarge) = 0.206663492640000D-013
Function calcQuakeGre:
thisInstance = 375
quakeGre(greSmall) = 0.289288522630000D-002
quakeGre(greMedium) = 0.100925919216016D-002
quakeGre(greLarge) = 0.134855070000000D-002

```

EXTANK Output Unit 2, Partial Listing

icase	GRE	rsg	trel	y1 max	tlurisk	tldrisk	y2 max	t2urisk	t2drisk
347	2	6.11269E-02	4684.810	0.085588	8.0709E+04	1.0182E+04	0.070484	2.5618E+03	0.0000E+00
347	3	5.50745E-03	70213.203	0.088213	1.4572E+05	3.5722E+04	0.000000	0.0000E+00	0.0000E+00
350	3	1.34436E-03	120476.000	0.029896	0.0000E+00	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
352	3	1.10761E-01	2413.740	0.080220	7.2892E+04	3.3073E+03	0.068361	1.6554E+03	0.0000E+00
353	2	1.10372E-02	16080.000	0.052034	3.8722E+04	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
353	3	5.39243E-02	17525.500	0.247200	1.9953E+05	1.2872E+05	0.234633	1.6584E+04	1.3162E+04
354	2	1.50449E-02	9441.750	0.043020	1.3031E+04	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
354	3	7.17900E-03	42742.000	0.079264	1.0754E+05	8.4864E+03	0.000000	0.0000E+00	0.0000E+00
355	3	5.71968E-02	2462.830	0.043398	1.0275E+04	0.0000E+00	0.027902	0.0000E+00	0.0000E+00
357	2	1.09452E+00	173.113	0.057783	3.8819E+04	0.0000E+00	0.047977	2.9958E+02	0.0000E+00
357	3	1.29362E-02	68004.000	0.202650	2.2681E+05	1.4381E+05	0.000000	0.0000E+00	0.0000E+00
358	3	7.30870E-01	512.281	0.109885	1.0350E+05	3.4945E+04	0.100683	1.5835E+03	4.6527E+02
359	2	9.61196E-04	265759.000	0.028399	0.0000E+00	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
359	3	3.28377E+00	184.052	0.169240	1.4657E+05	7.8156E+04	0.161105	2.0723E+03	1.0943E+03
360	3	3.72836E+01	32.964	0.304127	2.0516E+05	1.3679E+05	0.297923	2.8099E+03	1.8687E+03
361	3	1.66681E-01	2583.010	0.124908	1.1781E+05	4.8651E+04	0.114760	3.0649E+03	1.3343E+03
362	3	6.97679E-01	1171.380	0.219262	1.7335E+05	1.0479E+05	0.211620	3.2523E+03	2.1255E+03
363	2	8.76137E-03	24639.000	0.060730	6.2759E+04	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
363	3	3.45116E-03	244574.000	0.100148	3.3279E+05	1.9478E+05	0.000000	0.0000E+00	0.0000E+00
366	3	1.30380E-01	2352.300	0.091278	8.5944E+04	1.6561E+04	0.080066	2.0511E+03	9.8922E+01
369	3	2.03781E-01	1903.010	0.113501	1.0768E+05	3.8660E+04	0.103473	2.4279E+03	8.4200E+02
370	2	8.05675E-03	18099.199	0.042336	2.0083E+04	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
370	3	8.69885E-01	326.626	0.084958	7.7565E+04	9.0406E+03	0.075451	1.0369E+03	0.0000E+00
371	2	8.61361E-02	3350.960	0.086227	8.0732E+04	1.0831E+04	0.073470	2.2202E+03	0.0000E+00
371	3	5.98619E-01	645.386	0.113108	1.0649E+05	3.7895E+04	0.103883	1.7106E+03	5.5246E+02
374	3	8.95689E-02	1849.800	0.050779	2.6227E+04	0.0000E+00	0.037842	0.0000E+00	0.0000E+00
375	2	4.70765E-01	465.010	0.066351	5.2810E+04	0.0000E+00	0.056353	6.1632E+02	0.0000E+00
375	3	3.04876E-01	4254.160	0.316768	2.1305E+05	1.4424E+05	0.310231	6.5586E+03	5.1878E+03
378	3	6.85093E+00	91.627	0.174948	1.4982E+05	8.1427E+04	0.166924	2.0540E+03	1.0969E+03
379	3	9.14040E-02	2785.660	0.076603	6.8395E+04	0.0000E+00	0.063961	1.5889E+03	0.0000E+00
380	3	1.84849E-01	1244.570	0.069558	5.7911E+04	0.0000E+00	0.058724	9.0654E+02	0.0000E+00
381	3	8.27059E-04	350759.000	0.025495	0.0000E+00	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
383	3	1.80551E-03	118961.000	0.039889	1.1498E+05	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
385	3	7.41007E+00	26.388	0.059555	4.1800E+04	0.0000E+00	0.049949	3.3315E+02	0.0000E+00
386	3	9.37721E-04	261230.000	0.027609	0.0000E+00	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
388	3	1.46047E-01	1962.270	0.085649	7.9281E+04	1.0007E+04	0.074609	1.7072E+03	0.0000E+00
389	2	4.33217E-03	38067.102	0.043538	4.2855E+04	0.0000E+00	0.000000	0.0000E+00	0.0000E+00
389	3	1.44993E+00	122.183	0.054165	3.2319E+04	0.0000E+00	0.044376	1.7753E+02	0.0000E+00
391	3	1.91167E+00	182.416	0.102888	9.6684E+04	2.8243E+04	0.093777	1.2922E+03	2.8550E+02
393	3	2.91411E-02	10772.100	0.093287	9.3061E+04	2.0170E+04	0.051497	2.1130E+03	0.0000E+00
395	3	7.38628E-01	362.896	0.080417	7.2071E+04	3.5009E+03	0.070799	9.5277E+02	0.0000E+00
396	3	1.57976E+01	30.252	0.137315	1.2550E+05	5.7124E+04	0.128782	1.6493E+03	7.0333E+02

DISTRIBUTION SHEET

To	From	Page 1 of 1
D. R. Bratzel	Fluor Daniel Northwest	Date 6/15/98
Project Title/Work Order		EDT No. 619970
Gas Release Event Safety Analysis Tool/N23CD		ECN No. N/A

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
W. B. Barton	R2-12	X			
D. R. Bratzel (5)	S7-14	X			
M. J. Grigsby	S7-14	X			
B. E. Hey	B4-47	X			
G. D. Johnson	S7-14	X			
J. C. Lavender	K8-03	X			
E. R. Siciliano (5)	B4-43	X			
W. D. Wittekind	B4-44	X			
J. Young	S7-14	X			
Central Files (2)	B1-07	X			
RL Docket File (2)	A3-02	X			

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