Explosive Volume Formation from the Release of Vapors or Liquids in Enclosures

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ABSTRACT

Evaluation of the explosion hazard from accidental releases in enclosures involves estimating the flammable volume produced by mixing of the released material with air. Two specific situations are considered in the paper. In the first case dealing with gaseous jet releases, recent results are discussed on the effects of simple obstacles on the flammable volume. These results illustrate how the flammable volume can increase or decrease, depending on the values of dimensionless parameters that define the release and the obstacle. The second case considered is that of the flammable layer produced by the evaporation of a liquid pool. This particular release scenario has been studied using a computational approach based on a one-dimensional model. The paper discusses the rationale behind this approximation and the adjustments that have been found to be necessary to include multi-dimensional effects into the approximate treatment. The common thread among the correlations or calculation methods discussed in the paper is the desire to identify tools that can be of use in engineering applications.

KEYWORDS: jet releases, pool vaporization, stratified layers, flammable liquids

INTRODUCTION

A potential explosion hazard arises whenever the release of a combustible material (a liquid, gas or vapor) is followed by the formation of a flammable volume, as the released material mixes with surrounding air. The mixing process depends strongly on the conditions of the release and of the environment. The pressure and temperature of the storage or process containment from which the leak originates, and the size/shape of the break, fall within the first group of conditions. Factors such as the geometry of the room containing the leaking equipment, the obstacles in the path of the leak and ventilation are some examples of environment-related parameters. Efficient methods to estimate the influence of these various parameters are required for engineering analyses of the consequences of the release event.

Correlations have been developed to describe the behavior of releases under idealized conditions. However, more elaborate versions of these correlations, capable to account for certain complexities of the geometry of the system, are usually not available. For example, the case of a gaseous axisymmetric jet in unconfined surroundings is well documented in the literature. On the other hand, the modifications to the jet flow due to the impingement on obstacles are not well covered, at least not in any generalized fashion. The standard approach to the accounting of these more complex effects is by detailed

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numerical modeling of the particular geometry of the release configuration of interest. While the power and usefulness of computational fluid dynamics (CFD) tools is well recognized, these methods often do not provide the level of flexibility and user friendliness that is desirable for engineering tools.

This paper presents a review of results for the flammable volumes from simple releases. Some of these results consist of published correlations, while others introduce the findings of recent research. More specifically, the paper considers two types of releases: gaseous jets, both unconfined and impinging on obstacles, and layers produced by the vaporization of a liquid pool. Areas where additional research is needed are also highlighted.

TURBULENT FORCED JET RELEASES

Unconfined Axisymmetric Jet Flow

The situation considered here is that of the turbulent jet produced by a subsonic gas release from a circular orifice. In the absence of confinement, this type of release produces a self-similar flow after a distance of a few orifice diameters from the source. The variations of axial velocity and source material concentration in this asymptotic flow are described by well-known expressions. In terms of the volume fraction, X_i, and in the simpler case of a source fluid with density equal to that of the surroundings, these dependencies are formally written as [1,2]:

$$X_c - X_\infty = \left(X_0 - X_\infty\right)\left(0.185\,\frac{x}{D}\right)^{-1} \quad , \tag{1}$$

$$X - X_\infty = \left(X_c - X_\infty\right)\exp\left(-\frac{r^2}{b^2}\right) \quad \text{, and} \tag{2}$$

$$b = 1.201\, b_{1/2} = 0.127\, x \quad . \tag{3}$$

In these equations, the subscripts "*0*", "*c*" and "∞" indicate conditions in the source flow, on the centerline of the jet, and in the surrounding environment, respectively. The variable D is the initial diameter of the jet, while the quantity $b_{1/2}$ is the radial distance at which the concentration of the source material is equal to one half of its centerline value.

Modifications of these expressions have been introduced to account for the effects of source fluids of different density from that of the surrounding medium and for sonic releases. In the latter case, the jet is underexpanded at the nozzle exit (i.e., its pressure is still higher than that of the ambient) and further expansion takes place within a few diameters of the nozzle. This rather complex process is often approximated by assuming that the sonic release is equivalent to a subsonic jet originating from a nozzle with an equivalent diameter larger than the actual diameter by a factor that depends on the source pressure. While these adjustments may be required to deal with many practical applications, this level of complexity will be neglected in the following discussion.

Jet Flammable Volume

Mixtures of combustible gases with air are flammable (i.e., can support combustion) if the composition falls within a certain range, which is defined by the lower (LFL) and upper (UFL) flammable limits. In the case of a fuel release, only areas with concentrations

within this range will contribute to the flammable volume. For an unconfined jet, it is possible to obtain a simple expression for the volume, V_L, with concentrations above a certain value, X_L, by carrying out a double integral in the radial and longitudinal (r and x) direction of the composition field defined by Eqs. (1) - (3). The result is:

$$V_L = \frac{0.127^2 \cdot \pi}{0.185^3 \cdot 9} \left(\frac{X_0 - X_\infty}{X_L - X_\infty} D \right)^3 \quad . \qquad \textbf{(4)}$$

The constant term in the right-hand side of the equation (= 0.889) has been written in terms of the coefficients in Eqs. (1) and (3) so that it can be recalculated if different decay constants are preferred. Equation (4) indicates that the initial flow rate of source material is not an explicit factor. This is the case because, for a subsonic release, concentrations in the unconfined turbulent jet are independent of the velocity field. As a result, for a given break size, an increase in the exit velocity has no effect on the flammable volume of the jet. Another observation is the strong dependence of V_L on the diameter, D, of the jet.

While variations in the fuel concentration in the source fluid are of limited practical interest (this is typically 100%, i.e., $X_0 = 1$), the effect of the cutoff value, X_L, is worth discussing. In the case where no fuel has accumulated in the background ($X_\infty = 0$), the ratio between the two jet volumes, V_U and V_L, defined by the two cutoff concentrations, X_U and X_L, is:

$$V_U / V_L = \left(X_L / X_U \right)^3 \quad . \qquad \textbf{(5)}$$

Equation (5) shows that the volume of the jet with concentrations above the upper flammable limit is typically very small compared with the volume with concentrations above the LFL. In the case of methane, which has one of the lowest LFL/UFL ratios, the jet volume above the UFL is less than 4% of the volume above the LFL. This means that, in practice, the flammable volume of the jet can be calculated neglecting the rich mixtures and by simply using Eq. (4) with X_L set equal to the LFL concentration.

Volume of Source Material in the Jet

An analytical procedure analogous to that introduced in the preceding section can be used to calculate the volume of source material (fuel), which is present in the jet at concentrations above a certain cutoff, X_L. The result, which again applies under the simplified conditions introduced earlier (i.e., subsonic flow with no density effects), is:

$$V_{0,L} = \frac{0.127^2 \cdot \pi}{0.185^3 \cdot 9} \left(\frac{X_0 - X_\infty}{X_L - X_\infty} D \right)^3 \left(\frac{3}{2} X_L - \frac{1}{2} X_\infty \right) \quad . \qquad \textbf{(6)}$$

The ratio of Eqs. (6) and (4) yields an expression for the average concentration of source material in the jet volume at compositions above X_L. The expression for this ratio is:

$$V_{0,L} / V_L = \frac{3}{2} X_L - \frac{1}{2} X_\infty \quad . \qquad \textbf{(7)}$$

In the case of no fuel in the background ($X_\infty = 0$) and for X_L set equal to the LFL, this equation says that the average concentration in the flammable volume is 50% above the LFL. For many fuels, this implies a value approximately equal to 0.75 times the stoichiometric concentration. This result indicates that the reactivity of the volume is dominated by fuel concentrations below stoichiometric and, therefore, is less than what is normally assumed under simplified analyses relying on worst-case mixing models.

Effects of Obstacles

An increase of the fuel concentration in the background, X_∞, as would occur for a release inside an enclosure, has an impact on the flammable volume. The extent of the effect can be calculated from Eq. (4). Another manifestation of confinement is observed when the presence of an obstacle affects the very portion of the jet volume occupied by flammable compositions. This, of course, is the most likely practical situation, since releases involve equipment, which is typically in close proximity to other hardware or confining walls. The very broad range of possible geometric configurations, however, complicates the use of generalized treatments. Recently [3], a numerical study has addressed the impingement of an axisymmetric turbulent forced jet on simple obstacles. This study is of interest here because of its focus on the effect of the obstructions on the flammable volume in the jet.

The cited reference considered the situation where the obstacle is made of a disk placed perpendicular to and concentric with the axis of the jet, as shown in Fig. 1. This simple problem is characterized by four length scales, two of which relate to the jet itself (D and L_{LFL}) and two that define the obstacle (L_d and D_d). The length, L_{LFL}, is the distance from the jet origin at which the centerline concentration drops to the LFL value, when the obstacle is not present. It can be obtained by solving Eq. (1) for x, after having set $X_c = X_{LFL}$. The lengths, D_d and L_d, are the diameter of the disk and its distance from the origin of the jet.

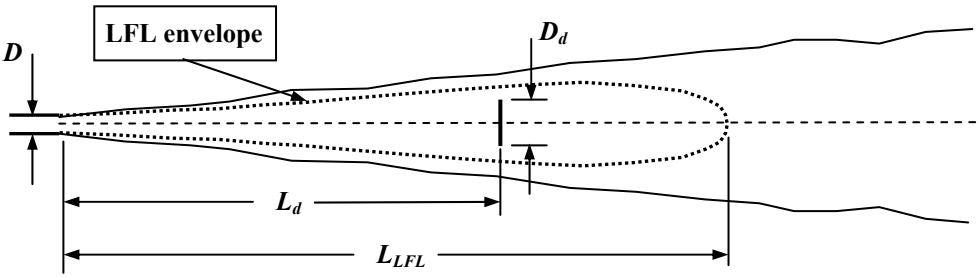

Figure 1 - Schematic View of Disk Obstacle Geometry for Jet Flow Calculations of Ref. [3].

The results of numerical calculations for the flammable volume, $V_{L,obs}$, with the disk obstacle in place are shown in Fig. 2. The predictions from the CFD code are normalized by the value of the flammable volume, V_L, for the unobstructed jet (cf. Eq. [4]). The abscissa in the plot is the obstacle radius, $D_d/2$, normalized by its distance from the jet origin, L_d. The parameter for the curves is the obstacle distance, L_d, divided by the "flammable" length, L_{LFL}, of the unobstructed jet. Predictions are shown for values of L_{LFL} corresponding to the two LFLs of 1.4 and 4%. As can be seen, the variations in this parameter are well correlated by the normalized presentation (overlap of open and solid symbols for the same L_d/L_{LFL}). Variations in jet diameter, D, have also been shown in Ref. [3] to be well correlated by the variables in Fig. 2.

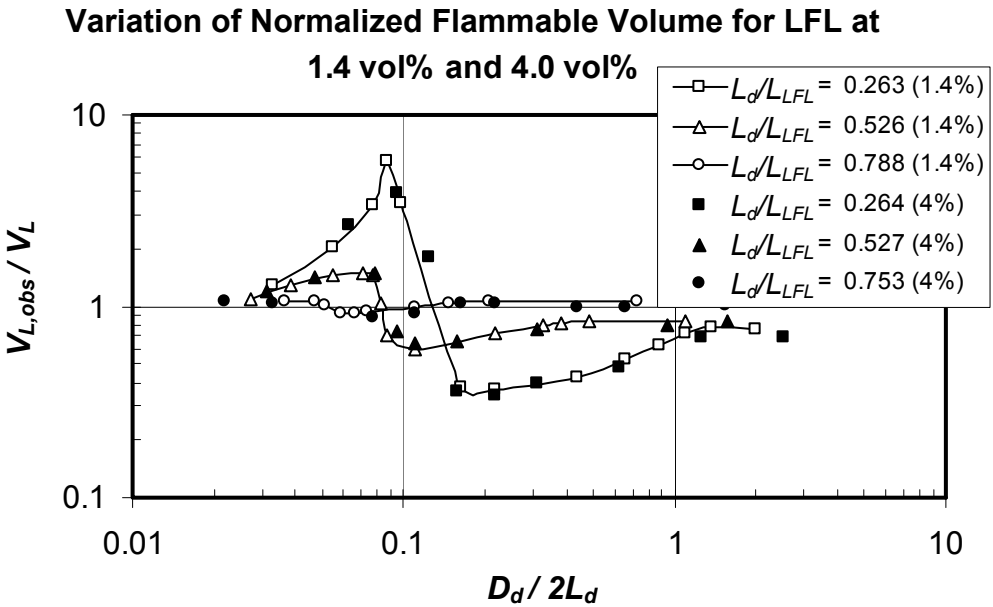

Figure 2 - Normalized Flammable Volume as a Function of Disk Size and Location in the Jet (taken from Ref. [3])

Several observations can be based on the results in the figure. First of all, it comes as no surprise that the effect of the obstacle, regardless of its diameter, decreases as its distance from the jet origin approaches the flammable jet length, L_{LFL}. On the other hand, for an L_d/L_{LFL} ratio of about 0.25, the effect of the obstacle becomes very significant, with the normalized flammable volume ranging from a three-fold drop to a seven-fold increase ($V_{L,obs}/V_L$ ranging from 0.35 to 7). A transition point clearly exists at a normalized obstacle size, $D_d/2L_d$, of about 0.1. As detailed in Ref. [3], this transition corresponds to a change in the nature of the flow associated with the presence of a recirculation zone (or lack thereof) behind the obstacle. Predictions are also reported in the same reference for the case of the jet impinging on a cylinder. These results, however, are only preliminary and have not been generalized to the extent of those of the simpler 2D case of Fig. 2.

LOW-PRESSURE GAS/LIQUID RELEASES

General Problem Description

Accidental leaks of flammable gases, vapors or liquids can occur under circumstances that facilitate the segregation of the released material. Mixing with surrounding air is promoted at a subsequent time by relatively slow diffusion mechanisms, which can be mainly laminar or can be assisted by the presence of natural or forced convection. An example of such a situation is the slow release of a heavy vapor near the floor of an enclosure. Another example is that of a flammable liquid spilled over the same floor. In the second situation, the mixing process must be preceded by vaporization of the liquid. In either case, high vapor concentrations develop first near the floor and lower values are found at increasing distances above the floor.

Work at FM Global Research has addressed the dispersion behavior of heavier-than-air flammable gases released near a floor and the combustion characteristics of the stratified layers formed as a result of the diffusion process [4]. These results are currently being used to develop an engineering tool to address the various aspects of the phenomenon as part of an integrated approach. The following discussion will focus on the component of this general solution which deals with the question of the flammable layer formation in the case of a vaporizing pool. With the exception of questions relating to the energy balance at the vaporizing surface, all other considerations also apply to the simpler case of slow dispersion of a heavy vapor injected near the floor.

Layer Formation Process

The vaporization of a flammable liquid and the creation of a fuel/air layer are well understood and relatively simple processes. The energy required for vaporization of the liquid is provided by conduction from the floor, heat transfer from the surroundings (by convection and radiation), and sensible heat of the spill. The evolution of the composition field in the gas phase is determined by convection and diffusion, which promote the mixing of the fuel vapors with surrounding air. At least conceptually, these processes are all within the predictive capabilities of available methods. Practical difficulties, however, can arise due to complexities in the geometry, presence of turbulence (from forced ventilation or natural convection), and discontinuities in the vaporizing surface (i.e., a pool not covering the entire floor area).

Unlike the case of forced jet release discussed earlier, there appear to be no simple general correlations describing this scenario, not even for the case in which the complicating factors mentioned above are absent. Rather than resorting to CFD models that provide a detailed description of the flow, an intermediate approach is introduced here, which takes advantage of the preferential nature of the vapor diffusion in this type of problem, involving heavier-than-air vapors. It is based on the simplifying assumption that the composition field is mostly characterized by variations in the vertical direction. Horizontal gradients are negligible by comparison. The main benefit of this one-dimensional treatment is that the numerical complexity of the analysis is dramatically reduced. Confirmation that horizontal mixing is fast was obtained in the propane diffusion tests described in Ref. [4]. As indicated, two factors can degrade the suitability of the one-dimensional approximation: a discontinuity at the pool edge and/or the presence of convective flows. Both aspects will be discussed further in the following sections.

Solution Method and Pool Boundary Condition

The model is based on the solution of the one-dimensional transport equations for energy (i.e., temperature, T, both in the gas phase and in the solid substrate) and species (i.e., fuel fraction, Y_f). When turbulent mixing is present, one additional equation is solved for the turbulence kinetic energy, k. Since the rate of pool vaporization per unit floor area, $\dot{m}_1''$, is not known *a priori*, the problem is addressed through an iterative process. This involves solving the two equations for T and Y_f while enforcing the energy balance at the vaporizing surface.

The treatment of the boundary condition at the pool surface is relatively straightforward when the liquid covers the entire floor area. In this case, the pool temperature, T_p, and the vapor mass fraction, Y_f, at the interface are uniquely defined from the solution of the energy and species transport equations. These two quantities are the required input to the relationship used to enforce the vapor equilibrium condition. The Clausius-Clapeyron equation sets a functional relationship between the vapor pressure, p_f, and the temperature, T_p. A form often used for this relationship is Antoine's equation, which reads:

$$\ln\left(p_f\right) = \mathrm{A} - \frac{\mathrm{B}}{\mathrm{C}+T_p} \quad , \qquad \textbf{(8)}$$

where A, B and C are empirical constants, whose values depend on the material considered and on the units used for p_f and T_p. The vapor pressure, p_f, is related to the vapor mass fraction, Y_f, through standard formulas that account for the molecular weights of the mixture components.

If the liquid covers only a fraction of the floor area, the condition given by Eq. (8) must be enforced with care, when property changes are only considered in the vertical direction, as is the case of the one-dimensional model introduced here. The assumption of negligible horizontal gradients, which becomes quite appropriate at a sufficient distance from the vaporizing pool, cannot describe the conditions near the floor. The fuel fraction at the vaporizing surface, $Y_{fw,z=0}$, is different from the average value of fuel mass fraction, $Y_{f,z=0}$, calculated at the floor by the one-dimensional model. The simplest possible approach would be to set these two concentrations to be equal. Physically, this is equivalent to assuming that horizontal diffusion takes place at an infinite rate everywhere. The second possibility would be to embrace the opposite extreme, by assuming no horizontal diffusion very close to the pool. Algebraically, this amounts to setting the vapor concentration, $Y_{fd,z=0}$, over the dry portion of the floor equal to zero. This, however, causes a problem if the vapors saturate the entire enclosure volume. In this limiting case, the asymptotic concentration in the volume would be equal to $Y_{f,z=0}$ ($= \alpha\ Y_{fw,z=0}$), instead of the correct limit of $Y_{fw,z=0}$ (α is the fraction of the floor covered by the pool).

In summary, the two simple treatments presented here would introduce different problems under different conditions. A better solution is to account, in an approximate fashion, for the fact that horizontal diffusion of vapors near the floor plays a role, whose importance depends on the specific conditions of the system. A sub-model that provides a reasonable simulation of this effect was, therefore, developed. A summary overview is presented in the following section.

Local Horizontal Diffusion

The sub-model is based on a simplified representation of the concentration field near the floor of the enclosure. Two different profiles are assumed to exist: one over the portion of the floor wetted by the pool; the other over the "dry" floor. The variables associated with these two profiles are, respectively, Y_{fw} and Y_{fd}. The solution provided by the one-dimensional diffusion calculation yields the vertical profile for the averaged fuel mass fraction, Y_f. By definition, this average concentration is related to Y_{fw} and Y_{fd} through:

$$Y_f = \alpha\, Y_{fw} + \left(1-\alpha\right) Y_{fd} \quad . \qquad \textbf{(9)}$$

Away from the floor, the two profiles of "wet" and "dry" concentrations eventually merge into one. At the lower elevations where the values differ, an inner core of heavy gas is

surrounded by lighter material. The sub-model postulates the existence of a transition region of height, h, over which horizontal diffusion equalizes the differences between the two profiles. This process involves the movement of fuel vapors from where they originate, i.e., above the vaporizing pool, to portions of the floor where there is no vaporization. This transfer of mass is due to a buoyancy-driven net flow, $\dot{m}_{exch}$.

The first step in the development of the sub-model is the derivation of an expression for the exchange flow, $\dot{m}_{exch}$, spreading out from the edge of the pool area. The equation used to calculate $\dot{m}_{exch}$ is:

$$\dot{m}_{exch} = u_{sl}\ \rho_w\ h \sqrt{4\,\pi\ A_{pool}} \quad . \tag{10}$$

This equation yields the mass exchange as the product between a velocity, u_{sl}, the density, ρ_w, of the layer, and the area of the cylindrical surface across which the mass transfer takes place. The velocity, u_{sl}, is calculated by postulating that buoyancy is the driving force for the slumping motion of a layer of heavy vapors. The process is described by using an expression [5] that has been found to accurately predict the spreading rate of a uniform layer into an environment also of uniform composition:

$$u_{sl} = \sqrt{a_g\ h \left(1 - \frac{\rho_d}{\rho_w}\right)} \quad , \tag{11}$$

where a_g is the acceleration of gravity and h is the height of the layer. The density ratio between the surrounding gas (ρ_d) and the spreading vapors (ρ_w) is calculated from the values of the fuel fractions over the dry and wet portions of the floor ($Y_{fd,z=0}$ and $Y_{fw,z=0}$).

The determination of the height, h, of the layer of heavy gas is addressed by noting that the concentration difference between the gas regions above the "wet" and "dry" floor reaches a maximum at $z = 0$ and decreases with height. The height of an equivalent layer of uniform composition is then defined based on the profile for the average vapor mass fraction, Y_f. The choice made in this selection is the height at which the average fuel mass fraction drops to the "dry" floor value, $Y_{fd,z=0}$. Analytically, the height of the slumping layer is finally calculated from the following expression:

$$h = \mathrm{c_h}\ \frac{\left(Y_f - Y_{fd}\right)_{z=0}}{\left|\partial Y_f / \partial z\right|_{z=0}} \quad . \tag{12}$$

Reasonable agreement with limited available data was obtained by setting $c_h = 0.2$.

The last assumption required for closure of the sub-model is one that relates the mass flow, $\dot{m}_{exch}$, to other known parameters of the problem. This is done by postulating that the flow of vapors leaving the edge of the pool area over height, h, balances the uniform vertical flow of vapors at height, h, over the "dry" floor area. In the final expression, the fuel mass fraction at the floor, $Y_{fd,z=0}$, is the only unknown. Since it cannot be solved explicitly for $Y_{fd,z=0}$, the equation is written in the following form that makes it amenable to a solution by iteration:

$$\left(Y_{f,z=0} - Y_{fd,z=0}\right)^2 = \frac{\dot{m}_1''\ \alpha\left(1-\alpha\right)}{\rho_w} \sqrt{\frac{A_{floor}\ Y_{f,z=0}^3}{4\,\pi\, a_g\, h_1^3\left(-\beta\right)}}\ \frac{\sqrt{1+\beta\, Y_{fd,z=0}}}{Y_{f,z=0} - \left(1-\alpha\right) Y_{fd,z=0}} \quad , \tag{13}$$

where $\beta\left(= M_a / M_f - 1\right)$ is a normalized density defect, A_{floor} is the floor area and $\dot{m}_1''$ is the average mass flux over that area.

With all these relationships in place, integration of the problem equations over a time step is now possible. The transport equations are solved for an assumed value of $\dot{m}_1''$. This yields a set of values for $Y_{f,z=0}$ and T_p. The fuel mass fraction over the dry floor ($Y_{fd,z=0}$) is then calculated from Eq. (13) and that over the wet floor ($Y_{fw,z=0}$) from Eq. (9). The process is repeated until a value of $\dot{m}_1''$ is found that yields a "wet" fuel fraction compatible with the equilibrium value associated with T_p. Two iterations after the first guess are generally found to be sufficient to yield a very accurate (1 part in 10^7) value of $\dot{m}_1''$ essentially over the entire calculation.

Comparison with Small-Scale Data

The experimental work reported in Ref. [6] provides data on the layer formation process, in terms of the time needed for the lower limit concentration to reach a certain height in the test vessel. This was determined as the earliest time at which repeated ignition attempts by a spark placed at a fixed elevation were observed to start combustion in the mixture above a liquid pool. The tests were carried out in a vessel 80 mm in diameter and 80 mm high. Ethanol was introduced at the bottom of the test volume into a 1-mm deep recess machined in the lower wall of the vessel. The area of this receiver was varied between 95, 25 and 6.25% of the area of the vessel. The temperature of the liquid was set equal to 294.5K. Presumably, the vessel was conditioned before the test to the same

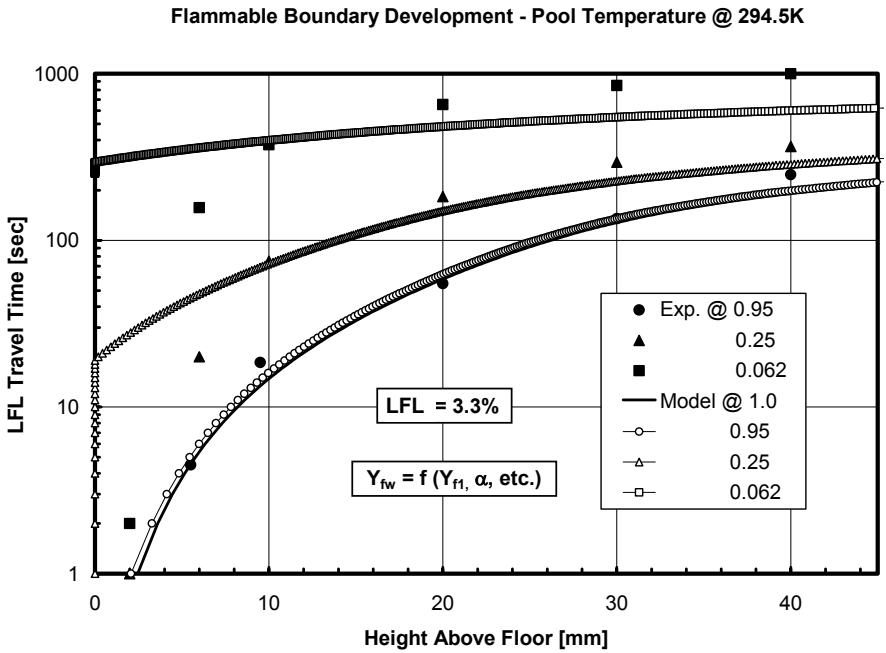

Figure 3 – Calculated and Measured Position of Upper Edge of Explosive Layer for Ethanol Vaporizing from a Pool Covering Different Fractions of the Floor Area (Data by Sato *et al*[6])

temperature as the liquid, but this detail remains unconfirmed.

A set of comparisons is shown in Fig. 3. This figure presents calculations and data for the arrival time of the upper boundary of the explosive layer for the liquid held at a constant temperature with the spill occupying different percentages of the enclosure floor surface. The model predictions are, in this case, strongly dependent on the simplifying assumptions introduced to deal within a one-dimensional treatment with an aspect of the problem which is definitely two-dimensional. The agreement between theory and experiment is reasonably good. In evaluating the results, it should be remembered that the data themselves contain two-dimensional effects, particularly at the low elevations. These would make the upper boundary of the explosive layer near the center of the enclosure travel faster than predicted by an average-flow calculation, due to the proximity with the vaporizing portion of the floor. In that sense, the fact that the model overpredicts the arrival times at heights lower than 10 mm can be attributed to the data more than to a failure of the model.

The result of the comparison at higher elevations is not as easily attributable to a data deficiency. In this case, the model predictions are moderately satisfactory. It should be noted, however, that the discrepancy is on the conservative side, with the model calculating arrival times that are shorter than measured in the experiments. In conclusion, while these considerations may fall short of a convincing validation, the model is considered acceptable for engineering purposes.

Ventilation

Forced ventilation affects the mixing inside an enclosure through two mechanisms: convective transport and turbulent diffusion. The established flow patterns are generally three-dimensional and not easily simplified. Despite this difficulty, the effect has been reduced to a one-dimensional treatment along the lines schematically shown in Fig. 4. The left half of the figure illustrates the part of the solution addressing the convective flow using a top in/bottom out configuration as an example. The entering flow is assumed to feed into the horizontal control slice near the ceiling, spanning the height of the inlet opening. Below that, the ventilation flow is constant and vertically downward all the way to the bottom control slice aligned with the height of the exhaust opening.

The other effect of ventilation is through production of turbulence, which increases diffusion. This is simulated by calculating the vertical variation of the turbulent field, assumed to be characterized by two properties: the turbulence kinetic energy, k, and the mixing length, L. The latter quantity is set equal to a prescribed constant fraction of the enclosure height, or to a linear function of distance from the nearest wall (floor or ceiling), whichever is smaller. The kinetic energy, k, is obtained by solving in one dimension a transport equation modeled following a standard approach documented in textbooks [7]:

$$\rho \frac{\partial k}{\partial t} + \rho w \frac{\partial k}{\partial z} = \frac{\partial}{\partial z}\left[\left(\mu + \frac{\mu_\tau}{\sigma_k}\right)\frac{\partial k}{\partial z}\right] + \rho\left(P_k - \varepsilon\right) \quad , \qquad \textbf{(14)}$$

where the terms P_k and ε represent the source and dissipation of turbulence kinetic energy. The turbulence viscosity, μ_τ, and the dissipation, ε, are given as functions of k and L by:

$$\mu_\tau = c_\mu^{\frac{1}{4}} \rho L k^{\frac{1}{2}} \qquad \text{and} \qquad \varepsilon = c_\mu^{\frac{3}{4}} \frac{k^{\frac{3}{2}}}{L} \quad . \qquad \textbf{(15)}$$

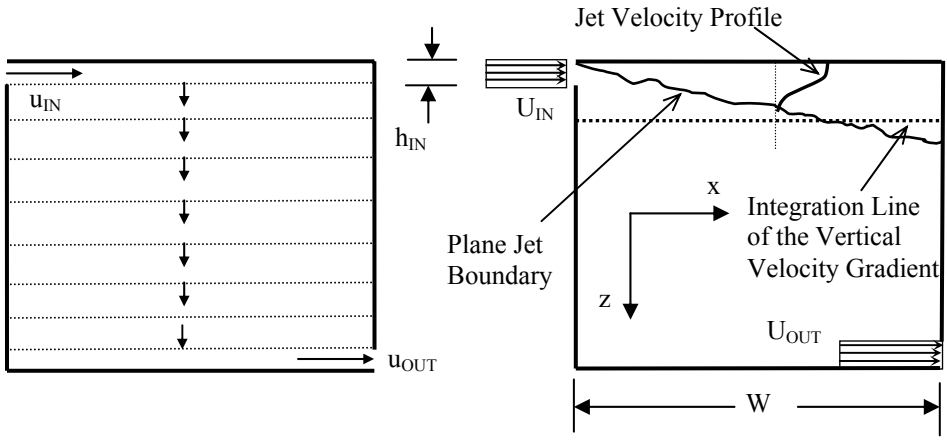

Figure 4 – Assumed One-Dimensional Representation of the Ventilation Flow (left side) and Free Jet Modeling of Turbulence Source (right side).

where c_μ is a constant (= 0.09). The effect of turbulent transport is included in the energy and species equation by adding μ_τ to the laminar viscosity in the diffusion term.

In the absence of buoyancy, the production of k is modeled by:

$$P_k = \frac{\mu_\tau}{\rho}\left(\frac{\partial u}{\partial z}\right)^2 \quad . \tag{16}$$

In this equation, generation of turbulence by shear is described by a term containing the average of the square of the vertical gradient of the horizontal velocity, $(\partial u/\partial z)^2$, produced by the ventilation flow. The analytical details leading to the algebraic expression for this gradient are beyond the scope of the paper. The general approach used in the derivation is shown schematically in the right side of Fig. 4.

The main assumption is that the ventilation flow can be represented as one half of a self-similar plane jet. The velocity distribution in the jet is then inferred from standard correlations and an approximate expression for the velocity gradient can be derived by integrating these correlations over horizontal lines. This provides the required source term for the turbulence transport equation as a function of height. By this approach, the two-dimensional turbulence source has been reduced to a one-dimensional equivalent. The reasonable character of the approximation was checked through comparisons with published results from numerical calculations for the flow situation depicted in Fig. 4. Horizontal averages were extracted from the two-dimensional predictions in Ref. [8] for the turbulence kinetic energy, k, and for the turbulent kinematic viscosity, $\nu_\tau = \mu_\tau/\rho$. The vertical variation of these two quantities was found to be in good agreement with the values calculated for the same flow conditions by the model introduced here.

It is recognized that the validation described above is limited and cannot be used as a rigorous test of the sweeping approximations introduced with the one-dimensional treatment. On the other hand, a more realistic model would impose computational requirements that exceed what can be conveniently accommodated by currently available

tools. Because of these limitations, the present approach should be considered appropriate to provide order-of-magnitude estimates of ventilation effects in scenarios involving slowly developing flammable layers. More sophisticated models should be developed to deal with situations where higher predictive accuracy is required.

SUMMARY AND CONCLUSIONS

The paper has addressed the question of predicting the extent of the flammable volume produced by accidental leaks of combustible vapors or liquids. The issue is relevant within the context of evaluations of the explosion hazard associated with these releases. Developments have been discussed for scenarios involving forced jets and layers from the vaporization of liquid pools. Recent results on the effect of simple obstacles on the flow pattern of the jet releases have shown that the flammable volume can be significantly affected. The adaptation of current knowledge on this type of release to practical problems still remains possible only if limited accuracy is expected. Additional research, particularly focused on the impact of more realistic obstructions, is needed.

The situations with regard to flammable liquid spills is somewhat more advanced. In this case, the impact on vapor dispersion of the details of the geometry is not as important and results obtained in simple configurations can be more easily generalized to real conditions. There is still a residual area of uncertainty with regard to ventilation. While a simplified one-dimensional approach is now available, its predictive capabilities are somewhat limited when complex forced or natural convection flows are present. More elaborate models will probably be required to achieve accurate estimates of these effects.

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