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**MODELING INDOOR DISPERSION OF AEROSOLS OR VAPORS
AND SUBSEQUENT VENTED FIRE OR EXPLOSION**

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Abstract

Considerable developmental work has gone into modeling dispersion of accidental outdoor releases; less has been applied to indoor releases. Indoor dispersion is characterized by the influence of a ventilation system and confining surfaces that facilitate aerosol rainout. Stratification can occur so that only part of a room contains flammable vapors, giving rise to so-called partial volume deflagrations. Indoor explosions are more complex to treat because there are two important regimes: before and after explosion vents, windows, or other panels open.

We describe here a model, WELMIX, to calculate time-varying concentration changes within a room from time-varying inputs such as occur with pool evaporation. The model allows for gas sensors in the room connected to automatic controls of the fresh air/recycle ratio and ventilation rate. We illustrate here the influence of ventilation rate and fresh air/recycle ratio on concentrations. A mixing efficiency is applied that is useful when the flammable vapors would not fill the entire room such as when the spilled material has low volatility.

We also describe two modules of the INVENT model to treat ignition of indoor vapor clouds. The INVENT model calculates the flame velocity, fireball growth with time, discharge rates, pressures, and temperatures inside and outside a room or dust bin. We concentrate here on the calculation of temperature and pressure before vents open.

Indoor Dispersion

Indoor dispersion has generally been treated as a well-mixed, first-order response system.

For example, general form solutions have been provided Glickman and Ujihara¹ and Shair and Heitner². Stratification of indoor concentrations was measured and modeled by Cleaver et. al.³ and Marshall⁴ releasing natural gas and propane. A parameter is defined by Cleaver et. al., the overturning number, that represents when the high momentum of a discharge or the buoyancy of a stratified layer will overcome tendencies to build up a stratified layer. In particular, spills of volatile liquids, evaporating with negligible momentum, can develop a concentration profile over the pool. The concentration profile can extend over the flammable concentration range as shown by carefully designed experiments using propane vapors by Tamanini and Chafee⁵.

Upon ignition, such low-lying profiles generally accelerate to deflagrations. If obstacles are present in the room the flames may accelerate to more damaging speeds. Tamanini and Chafee provide a correlation for explosion vent area requirements from such an explosion, termed a partial-volume-deflagration (PVD) since only part of the room volume contains vapors in the flammable concentration range.

There is a need for an indoor discharge model that can at least approximate the conditions leading to a PVD. It is also desirable to treat the important variables in a ventilation system, namely the ventilation rate as air changes per hour and the fresh air makeup ratio. We have developed a model to address these needs: the WELMIX model. As Figure 1 illustrates, the WELMIX model accounts for recirculating ventilation with a variable fraction of fresh air to recirculated air, f_a . It accepts time-varying source rates as developed by a pool spread and evaporation model. The program allows a gas sensor system to automatically vary the mass ventilation rate F_{in} (or volumetric air changes/hour, N_{ch}) and/or fresh air fraction when the predicted concentrations reach pre-defined alarm points. This allows various mitigation strategies based on gas sensors to be tested. The WELMIX model provides a mixing efficiency factor, η , that models part of the room as either a dead zone, bypassed by the ventilation air, or as a bypass zone in which part of the ventilation air does not mix with the source. In the dead zone model, the flow through the top part of the room is zero (the schematic valve is closed). For the bypass model, the fraction $(1-\eta)F_{in}$ of the ventilation flow passes through the top, bypass section of the room.

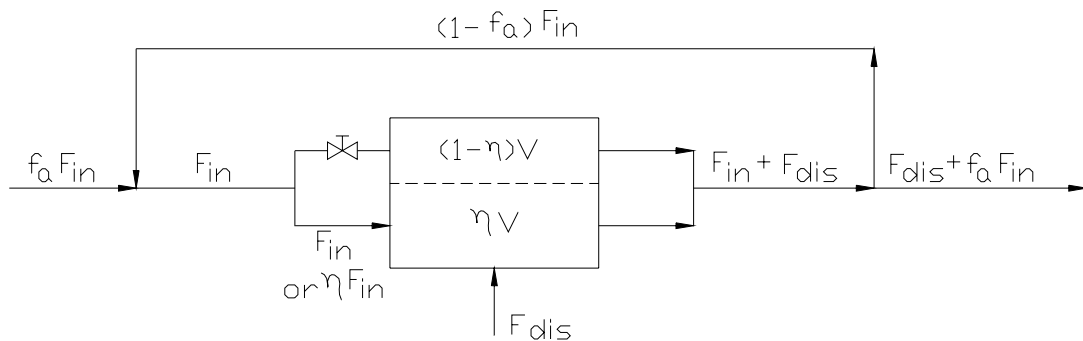


Figure 1 Schematic of Room Ventilated with Recycle System, Mass Balance

Indoor Dispersion Model Theory

A discharge inside a room of volume V with air density ρ injects a time-varying rate, F_{dis} , of contaminant with mass fraction, $w_{c,dis}$. The overall mass balance on a room for either the dead zone or the bypass model is given by:

$$V \frac{d\rho}{dt} = F_{in} + F_{dis} - F_{out} \quad (1)$$

The two specified rates are F_{dis} and the mass ventilation rate F_{in} . Expressing the ventilation rate in terms of the number of air changes/hr, N_{ch} , gives:

$$F_{in} = \frac{V \rho N_{ch}}{3600} \quad (2)$$

Assuming steady state in the ducts, pressures and flows will be constant. The flow at the nodes (mixing or branching points) adds to zero, so the overall mass balance is as shown in Figure 1. The steady-state component mass balance is shown in Figure 2, with the same steady-state assumption in the ducts. The unsteady-state component mass balance on the room differs slightly for the bypass model and dead zone models. Mass fractions are denoted w_c .

For dead zone model

$$\eta V \frac{dw_c}{dt} = F_{in} w_{c,in}(t-t_d) + F_{dis} w_{c,dis} - (F_{in} + F_{dis}) w_c \quad (3a)$$

For bypass model

$$\eta V \frac{dw_c}{dt} = \eta F_{in} w_{c,in}(t-t_d) + F_{dis} w_{c,dis} - (\eta F_{in} + F_{dis}) w_c \quad (3b)$$

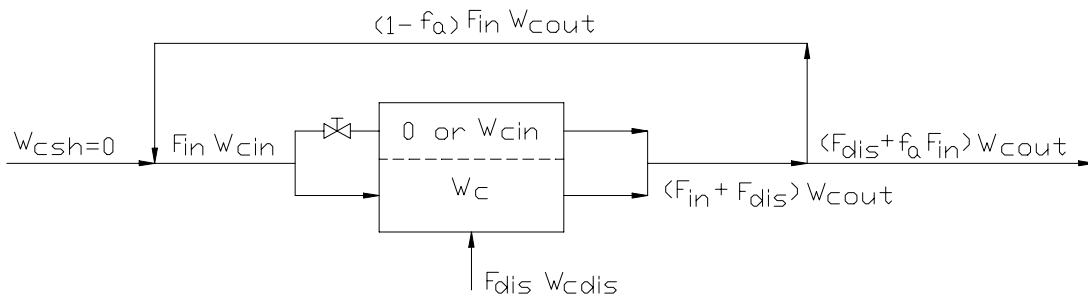


Figure 2- Steady-State Component Mass Balance on Room

At the right-hand node (split of exhaust and recycle), the component balance is:

For bypass model

$$(1-\eta)F_{in}w_{cin} + (\eta F_{in} + F_{dis})w_c = (F_{in} + F_{dis})w_{cout} \quad (4a)$$

and after some algebraic manipulation:

$$w_{cout} = \frac{(\eta F_{in} + F_{dis})w_c}{F_{dis} + F_{in} \left[1 - (1-\eta)(1-f_a) \right]} \quad (4b)$$

Similarly,

For dead zone model

$$(F_{in} + F_{dis})w_c = F_{out}w_{cout} \quad (5a)$$

$$w_c = w_{cout} \quad (5b)$$

Thus, the dead zone model is considerably simpler than the bypass model. Eliminating w_{cout} in Eq. 3 reduces the unsteady-state component mass balance on the room to a linear ordinary differential equation:

For dead zone model

$$\frac{dw_c}{dt} + \left[F_{in} + F_{dis} - (1-f_a)F_{in} \right] \frac{w_c}{\eta V \rho} = \frac{F_{dis}w_{cdis}}{\eta V \rho} \quad (6a)$$

For bypass model

$$\frac{dw_c}{dt} + \frac{(\eta F_{in} + F_{dis}) \left[F_{dis} + f_a F_{in} \right]}{F_{dis} + F_{in} \left[1 - (1-\eta)(1-f_a) \right]} \frac{w_c}{\eta V \rho} = \frac{F_{dis}w_{cdis}}{\eta V \rho} \quad (6b)$$

These are linear differential equations with constant coefficients in the form of a time constant, τ which has a solution:

$$w_c(t-t_o) = w_c(t_o)e^{-\left(\frac{t-t_o}{\tau}\right)} + w_{cmax} \left[1 - e^{-\left(\frac{t-t_o}{\tau}\right)} \right] \quad (7)$$

where w_{cmax} is the new steady-state value reached when the time interval $(t-t_o)$ is large.

The coefficients are:

For dead zone model

$$w_{C_{\max}} = \min \left\{ \begin{array}{l} \frac{F_{dis} w_{cdis}}{F_{dis} + f_a F_{in}} \\ 1 \end{array} \right. \quad (8a)$$

$$\tau = \frac{\eta \rho V}{F_{dis} + f_a F_{in}} \quad (8b)$$

For bypass model

$$w_{C_{\max}} = \min \left\{ \begin{array}{l} \frac{F_{dis} w_{cdis} \left\{ F_{dis} + F_{in} \left[1 - (1 - \eta)(1 - f_a) \right] \right\}}{\left(F_{dis} + \eta F_{in} \right) \left(F_{dis} + f_a F_{in} \right)} \\ 1 \end{array} \right. \quad (9a)$$

$$\tau = \frac{\eta \rho V \left\{ F_{dis} + F_{in} \left[1 - (1 - \eta)(1 - f_a) \right] \right\}}{\left(F_{dis} + \eta F_{in} \right) \left[F_{dis} + f_a F_{in} \right]} \quad (9b)$$

The room density, ρ , and so the time constant, τ , vary slightly, but the solution remains approximately valid. The step size for print-out, Δt , for this analytical solution can be as large as desired.

Finding Time to Reach Alarm Points

The time to reach a specified concentration such as the low and high alarm points, can be defined by:

t_1 = time to reach lower alarm point, $w_{c_{low}}$, by increasing concentration, s.

t_2 = time to reach upper alarm point, $w_{c_{hi}}$, by increasing concentration, s.

t_3 = time to reach lower alarm point, $w_{c_{hi}}$, by decreasing concentration, s.

t_4 = time to reach lower alarm point, $w_{c_{low}}$, by decreasing concentration, s.

These times are readily found by solving for time from Eq. 7.

The output is provided as both mole fraction and mass fraction with time. Mole fraction is found as:

$$y_i = w_i \frac{M_{mix}}{M_i} \quad (10)$$

where the multicomponent mixture molecular weight, M_{mix} , is given in terms of the mass fractions, w_i , and the component molecular weights, M_i , by:

$$\frac{1}{M_{mix}} = \sum_i \frac{w_i}{M_i} \quad (11)$$

Examples of Indoor Concentration Model Predictions

To show the nature of the WELMIX model predictions, Figure 3 uses an arbitrary step function for the source rate and extreme values for the ventilation rate. Figure 3 illustrates that the concentration follows the source rate, decaying to zero when the source rate stops. Each step increase in the source rate generates a new value of the ultimate maximum concentration, w_{cmax} , and correspondingly, mole fraction, y_{cmax} . Yet, the concentration is unable to reach each new y_{cmax} because the time-constant is relatively large compared with the step durations. Increasing the ventilation rate at 240 seconds drives down the concentration. The parameters used for Figure 3 are an acetone release with a room size of 200 m^3 , an ambient temperature of 27 C , a fresh air makeup ratio of 1, and a mixing coefficient of 1, so both the bypass and the deadzone models give the same results. The thresholds for increasing the ventilation rate are as follows:

Threshold (Fraction of LFL)	Threshold (Mole % Acetone)	Vent. Rate (ACH)
0	0	50
0.05	0.13	150
0.75	1.95	500
1	2.6	--

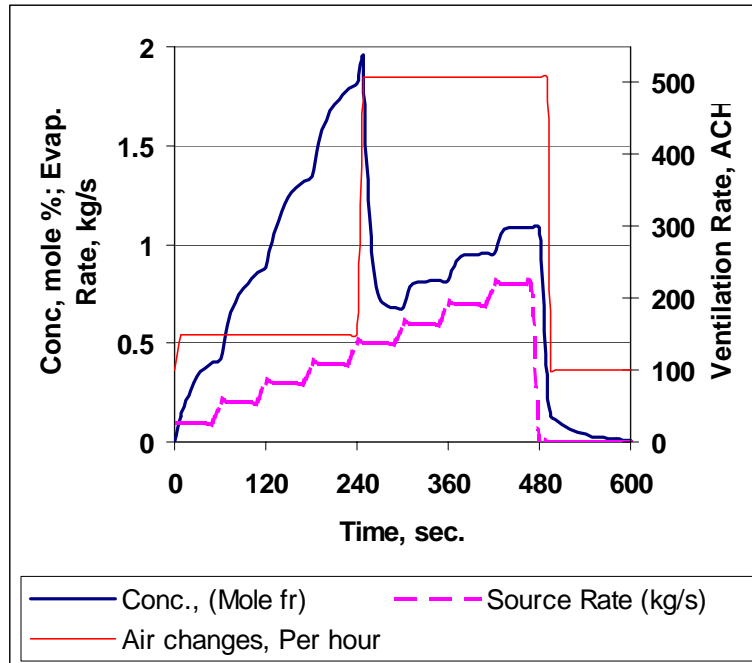


Figure 3 Illustration of Nature of Solution With Arbitrary Step Function Source Rate of Acetone and Unusually High Ventilation Rates

The second example, in Figure 4, is for a propane spill in a room of 400 m^3 volume with 6 air changes/hour (ACH). Again no stratification is assumed, so the mixing efficiency is 1. The source rate is 0.05 kg/s for 900 s. and 0.065 kg/s for the next 900 s. In this case, the fresh air makeup rate is changed from 0.3 to 1.0 if the room concentration reaches 50% of the LFL or 1.05 mole %. The increase in fresh air makeup fraction occurs early in the response, and reduces the room concentrations from the upper dashed curve to the lower solid line. Thus, the peak room concentration is reduced by about 1/2, but for the strong source rate postulated the concentrations exceed the LFL of 2.1% in each case. Increasing the ventilation rate can further reduce concentrations.

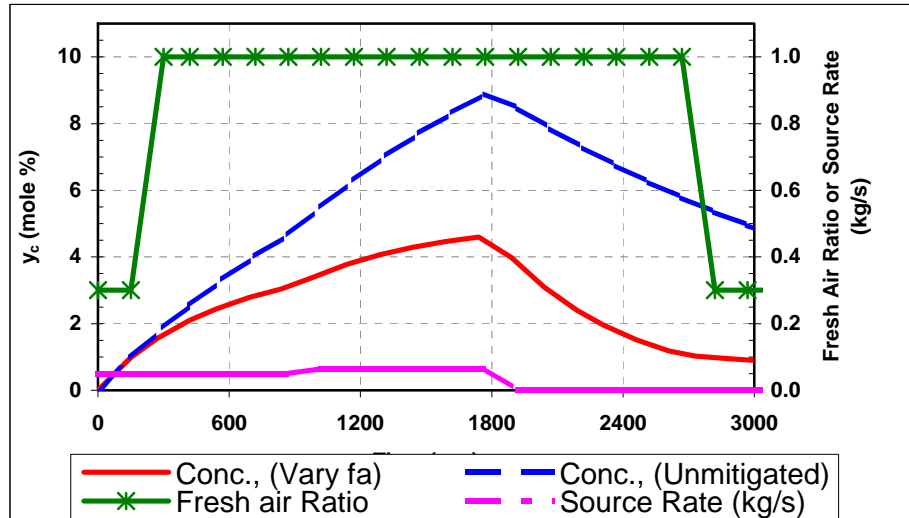


Figure 4 Illustrating the Influence of Changing the Fresh Air Makeup Alone

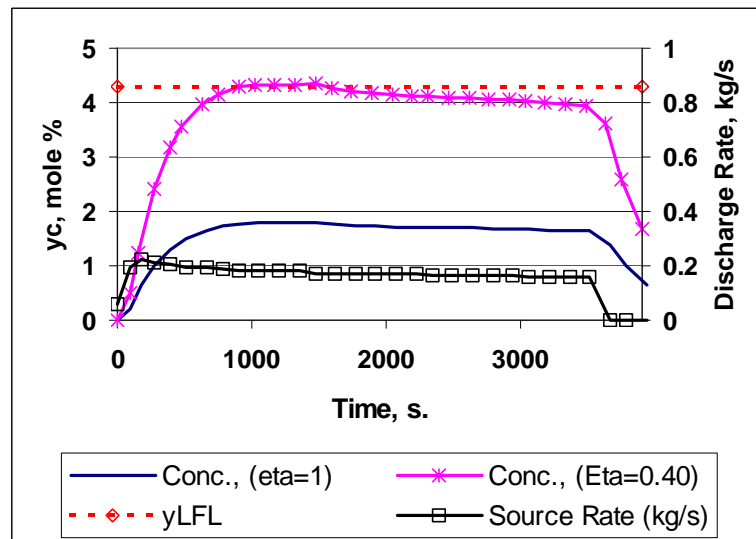


Figure 5 Illustration of Finding the Maximum Fraction of a Room That Could Contain a Flammable Mixture With Stratification

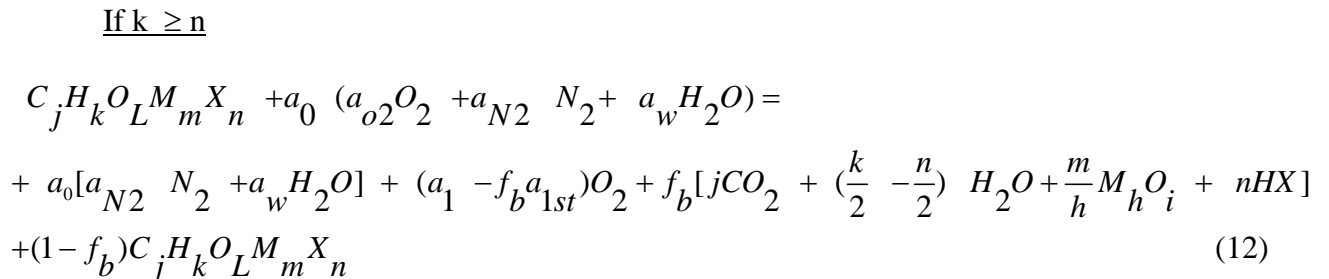
The third example, shown in Figure 5, illustrates how the effect of possible stratification can be investigated using the mixing efficiency factor. We postulate a spill of relatively low-volatility ethanol in a fairly large volume laboratory of 1800 m³ under a hot summertime temperature of 35 C, with a constant 10 ACH. A large pool size is conservatively postulated, giving the substantial source rate plotted as the bottom curve against the right-hand scale in Figure 5. If the vapors are assumed to be well-mixed in the entire room volume, the predicted concentrations follow the lower concentration curve. These concentrations fall considerably below the LFL of 4.3 mole % plotted as the upper dashed line. If we postulate a value $\eta = 0.4$,

using the bypass-model, the upper concentration curves results, which just reaches the LFL for a brief period. Thus, the model enables an estimate that for these specific conditions, the maximum room volume that could contain flammable vapors with highly-stratified heavy vapors would be 40%. Such estimates provide the inputs to a model for partial-volume deflagrations discussed next.

Modeling Indoor Fire and Explosion

Unfortunately, indoor explosion modeling is not as well advanced as outdoor explosion modeling, has less experimental basis. Design correlations such as NFPA 68⁶ do not account for low volatility materials such as ethanol that produce conditions well below the worst-case assumed condition of a room full of gas at its stoichiometric concentration. Neither does NFPA 68 account for congestion such as pumps and vessels inside the building that can increase overpressures by flame acceleration.

The first step in modeling an indoor fire or explosion is to calculate the temperatures developed as a flame front burns a pre-mixed cloud. To do so, we make use of the stoichiometric formula for burning a general fuel which can be a vapor, aerosol, or dust. The formula for incomplete combustion of a generic fuel with the formula $C_jH_kO_LM_mX_n$ in moist air is:



where M is a generic metal (such as sulfur, S, phosphorus, P, Lithium, Li, etc., and X is a generic halide (F, Cl, Br, or I) and here we define dry air as a two-component mixture of nitrogen and oxygen.

The coefficients are:

$$a_0 = \text{moles of dry air/mole of fuel} \tag{13a}$$

$$a_{O_2} = \text{moles of oxygen/mole of dry air} = 0.20946 \tag{13b}$$

$$a_1 = \text{moles oxygen/mole of fuel} \quad (13c)$$

so

$$a_1 = a_{O_2} a_0 = 0.20946 a_0 \quad (13d)$$

$$a_{N_2} = \text{moles of nitrogen/mole of dry air} = 0.79054 \text{ in two-component air} \quad (13e)$$

$$a_{1st} = \text{stoichiometric moles of oxygen/mole of fuel} \quad (13f)$$

$$a_{1st} = j + \frac{k}{4} - \frac{n}{4} + \frac{i m}{2 h} - \frac{L}{2} \quad (13g)$$

$$a_{0st} = a_{1st} / a_{O_2} \quad (13h)$$

$$a_w = \text{moles of water/mole of dry air components} = \frac{y_w}{1 - y_w} \quad (13i)$$

The mole weight of humid air is given by:

$$M_{wair} = (1 - y_w) M_{da} + y_w M_w \quad (14)$$

using M_{da} for the mole weight of dry air. The mole fraction of water in air is found from the

relative humidity, RH, and the saturation pressure of water, P_w in atmospheres, or:

$$y_w = RH P_w(T) / P_a \quad (15)$$

When the number of hydrogen atoms is insufficient to form HX with all the halide, molecular halide is found to form. We ignore this case.

The mass or mole fraction of fuel burned, f_b is limited by the availability of fuel or air so:

$$f_b = \max \left\{ \begin{array}{l} 1 \text{ if } \frac{a_0}{a_{0st}} > 1 \\ \frac{a_0}{a_{0st}} \text{ if } \frac{a_0}{a_{0st}} \leq 1 \end{array} \right\} \quad (16)$$

The mass air to fuel ratio, a_f , is related to the excess air fraction, x_s , by:

$$\frac{a_1}{a_{1st}} = \frac{a_0}{a_{0st}} = \frac{a_f}{a_{fst}} = (1 + x_s) \quad (17)$$

Here, x_s is the ratio of the mass of air in excess of the stoichiometric air to the stoichiometric air mass rate m_{airst} . The mass rate of air to the plume, m_{air} , is:

$$m_{air} = (1 + x_s) m_{airst} \quad (18)$$

In a fuel-rich mixture, the actual to stoichiometric ratio in Eq. 17 is less than 1, x_s is < 0 , so x_s is bounded only on the low side:

$$-1 \leq x_s$$

Mass Balance In Fire

The mass balance per mole (or per mole/s) of fuel follows the stoichiometric equation with each term multiplied by the respective molecular weights, M_i (for $k \geq n$):

$$M_{fuel} + a_o(M_{da} + a_w M_w) = a_o [a_{N2} M_{N2} + a_{bal} M_{bal} + a_w M_w] + a_{O2} (a_o - f_b a_{0st}) M_{O2} + f_b [j M_{CO2} + \left(\frac{k}{2} - \frac{n}{2} \right) M_w + \frac{m}{h} M_{ox} + n M_{HX}] + (1 - f_b) M_{fuel} \quad (19)$$

The mass ratio of moist air per mass of fuel initially present, a_f is:

$$a_f = \frac{a_o(M_{dair} + a_w M_w)}{M_{fuel}} \quad (20)$$

So, the rate of air entrainment to the plume is the air/fuel ratio times the initial fuel rate, m_{f0} :

$$m_{air} = a_f m_{f0} \quad (21)$$

The total mass rate in the plume equals the mass rate of fuel plus air:

$$m_{plume} = (1 + a_f) m_{f0} \quad (22)$$

Combining Eqs. 13i, 14, and 20 gives:

$$a_f = \frac{a_o M_{wair}}{(1 - y_w) M_{fuel}} \quad (23)$$

and, after some manipulation:

$$\frac{a_o}{a_{0st}} = \left(\frac{y_{fst}}{1 - y_{fst}} \right) \frac{(1 - y_f)}{y_f} \quad (24)$$

This relates the mole fraction of fuel to the fuel/air coefficients.

Enthalpy Balance in Fire

The enthalpy balance follows directly from the mass balance, Eq. 13, and has units of J/mole of fuel initially present. The left-hand side (LHS) of the enthalpy balance adds the enthalpy of initial fuel, entrained air, and heat of combustion. This must equal the enthalpy of the products of combustion on the right-hand side (RHS). The enthalpy balance is:

$$\begin{aligned}
& M_f H_f(T_0) + a_o [M_{da} H_{da}(T_{amb}) + a_{bal} M_{bal} H_{bal}(T_{amb}) + a_w M_w H_w(T_{amb})] + \\
& f_b M_f H_{comb}(1 - f_{rad}) \\
& = a_o [a_{N2} M_{N2} H_{N2}(T_f) + a_w M_w H_w(T_f)] + a_{o2} (a_o - f_b a_{ost}) M_{O2} H_{O2}(T_f) \\
& + f_b [j M_{CO2} H_{CO2}(T_f) + (\frac{k}{2} - \frac{n}{2}) M_w H_w(T_f) + \frac{m}{h} M_{ox} H_{ox}(T_f) + n M_{HX} H_{HX}(T_f)] \\
& + (1 - f_b) M_f H_f(T_f) \tag{25}
\end{aligned}$$

In the case of an evaporating liquid fuel, the fuel enthalpy on the LHS is found relative to a basis enthalpy of liquid at ambient temperature. Some of the heat of combustion is used to elevate the liquid enthalpy, H_{Lf} , from the initial temperature, T_{in} to the normal boiling point, T_{nbp} , and to supply the heat of vaporization, h_{fg} , so:

$$H_f(T_0) = H_{Lf}(T_{in}) - \Delta H_{Lf}(T_{nbp} - T_{in}) - h_{fg}(T_{nbp}) \tag{26}$$

Use the enthalpy balance to find the temperature of the plume as a function of excess air. This is done by a root-finding routine. The reactant enthalpies are all evaluated at the ambient temperature, T_a . The product enthalpies are all evaluated at the postulated fire temperature T_f . We used the AIChE DIPPR system⁷ for physical properties. The range of validity for the enthalpy routine varies with components, but is around 900 to 1500 K. Above 1500 K we hold the heat capacity constant and extrapolate using $\Delta H = C_p \Delta T$. The Brent root finder routine varies T_f until the value of the enthalpy function, H_{net} is near to zero, where:

$$H_{net} = H_{reac} - H_{prod} \tag{27}$$

The enthalpy of moist air is made up of that of dry air and water:

$$H_{air} = a_o (M_{dair} H_{dair} + a_w M_w H_w) \tag{28}$$

Fire Temperature Profiles

An example of the fire temperatures predicted using the enthalpy balance is shown in Figure 6 for methane and ethanol fires. This illustrates the effect of radiated heat in lowering the flame

temperature. In a pool fire as much as 35% of the energy radiates from the fire. In an explosion, only about 5% of the energy is lost by radiation, so F_{rad} is set to 0.05. Setting F_{rad} to zero gives the top curve, which gives the reported values for adiabatic flame temperature as measured in a calorimeter. The flame temperature is lower for ethanol than for methane.

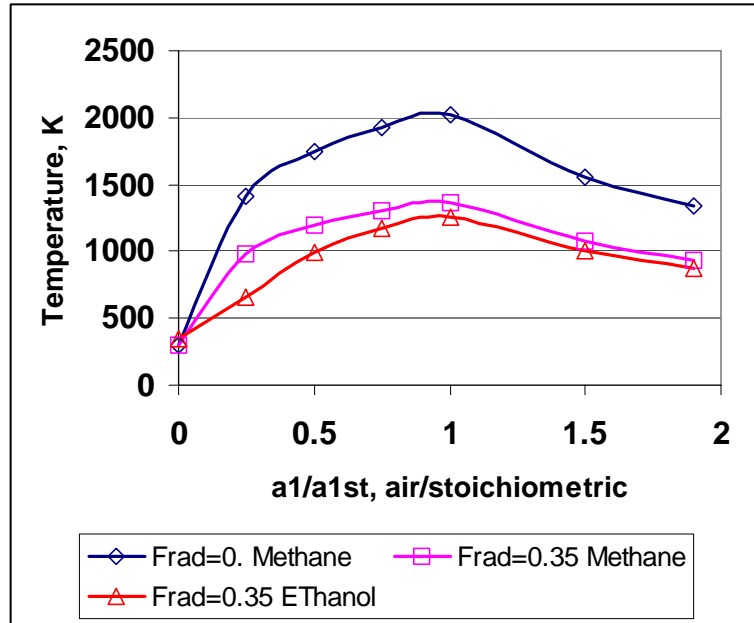


Figure 6 Example of Flame Temperatures Calculated Using Enthalpy Balance

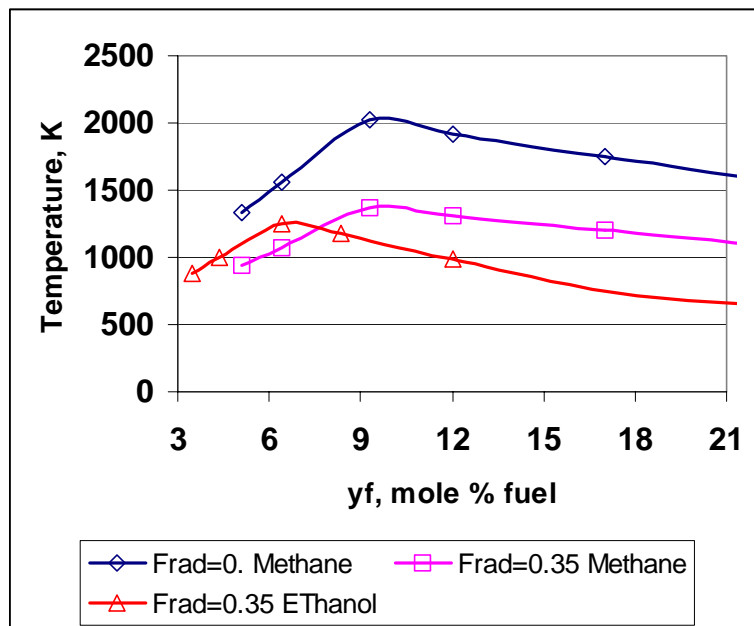


Figure 7 Flame Temperature Plotted Against Fuel Concentration

Figure 7 transforms the abscissa coordinate using Eq. 24 to plot temperature against fuel concentration. Since the stoichiometric concentration varies with fuel, the peak temperature also varies with fuel type when plotted against y_f .

Modeling Pressure From Partial Volume Combustion

The next step in modeling indoor combustion is to calculate the equilibrium pressure resulting from the combustion. A general situation is that of a small vapor cloud within a much larger enclosure, called a partial volume combustion. Consistent with the assumptions of the WELMIX model, we next calculate the pressure developed by igniting a room with an initial fraction of the room volume, $\eta_1 V$, filled with vapors above the LFL. This is done in two steps, using either of two alternative assumptions: (1) combustion at constant pressure, followed by adiabatic compression; or (2) combustion at constant volume, followed by adiabatic compression. That is:

Isobaric Solution

1) Burn the combustible volume $\eta_1 V$ at constant initial pressure, P_1 . Call this volume the “hot side” and the noncombustible volume $(1-\eta_1)V$, the “cool side”. Find the temperature, T_{h2} , and average molecular weight, M_{h2} , of the hot side combustion products using the fire enthalpy balance. The hot side density at this temperature and pressure will be too low, so the calculated volume of combustion products will generally exceed the room volume.

2) Expand the hot side and compress the cool side adiabatically until the pressure, temperature, and density of each is consistent with mass and volume balance.

Isochoric Solution

1) Burn the combustible volume $\eta_1 V$ at constant volume. Calculate the pressure required to keep the hot gases at constant volume, P_{h2} .

2) Expand the hot side and compress the cool side adiabatically until the pressure, temperature, and density of each is consistent with mass and volume balance.

In both cases, we assume the thermodynamic path moves through three states: 1) initial conditions, 2) compressed or uncompressed combustion products, 3) expanded conditions. The equations describing these states are given below.

Initial Conditions, State 1

Designating the portion with combustibles with subscript h (hot side) and the other with subscript c (cool side), the initial mass in each portion of the room is given by:

$$m_{h1} = \rho_{h1}V_{h1} = \rho_{h1}\eta_1V \quad (29a)$$

$$m_{c1} = \rho_{c1}V_{c1} = \rho_{c1}(1-\eta_1)V \quad (29b)$$

where the volumes and density are defined in terms of the ambient temperature, T_1 , ambient pressure, P_1 , and molecular weights of humid air, M_{wair} and of the fuel/air mixture, M_{h1} by:

$$V_{h1} = \eta_1V \quad (30a)$$

$$V_{c1} = (1-\eta_1)V \quad (30b)$$

$$\rho_{h1} = \frac{M_{h1}}{22.414} \frac{273.15}{T_1} \frac{P_1}{1.01325} \quad (31a)$$

$$\rho_{c1} = \frac{M_{wair}}{22.414} \frac{273.15}{T_1} \frac{P_1}{1.01325} \quad (31b)$$

Combustion Products, State 2, Isobaric Solution

After combustion at constant pressure, the fire model described above provides the temperature and molecular weight of the combustion products, T_{h2} and M_{h2} . Conserving mass and using the ideal gas density gives the hot side volume, V_{h2} . This volume may be larger than the available volume, that is the “fraction” η_2 may be > 1 . This unrealistic condition is rectified in State 3.

$$\rho_{h2} = \frac{M_{h2}}{22.414} \frac{273.15}{T_{h2}} \frac{P_1}{1.01325} \quad (32a)$$

$$V_{h2} = \frac{m_{h2}}{\rho_{h2}} = \eta_2V \quad (32b)$$

Combustion Products, State 2, Isochoric Solution

With the assumption of constant volume burning:

$$V_{h2} = V_{h1} \quad (33a)$$

and by ideal gas density, the pressure required is:

$$P_{h2} = P_1 \frac{T_{h2}M_{h1}}{T_{h1}M_{h2}} \quad (33b)$$

Compressed Conditions, State 3, Isobaric Solution

After combustion, the hot side will expand and compress the cold side, achieving a new volume fraction, η_3 . Since mass is conserved in each side, the new densities are:

$$\rho_{h3} = \frac{m_{h1}}{\eta_3 V} \quad (34a)$$

$$\rho_{c3} = \frac{m_{c1}}{(1 - \eta_3)V} \quad (34b)$$

The standard adiabatic, isentropic compression formula relates density, temperature, and pressure, so temperature and pressure can be found from the known densities using:

$$P_{h3} = P_{h2} \cdot \left(\frac{\rho_{h3}}{\rho_{h2}} \right)^{\gamma_h} \quad (35a)$$

$$P_{c3} = P_{c1} \cdot \left(\frac{\rho_{c3}}{\rho_{c1}} \right)^{\gamma_c} \quad (35b)$$

$$T_{h3} = T_{h2} \cdot \left(\frac{\rho_{h3}}{\rho_{h1}} \right)^{\gamma_h - 1} \quad (35c)$$

$$T_{c3} = T_{c1} \cdot \left(\frac{\rho_{c3}}{\rho_{c1}} \right)^{\gamma_c - 1} \quad (35d)$$

where:

γ_h = Specific heat ratio (C_p/C_v), for the combustion products, averaged over temperature range T_1 to T_{h3} .

Similarly, γ_c is the specific heat ratio for air averaged over the temperature T_1 to T_{c3} .

The density used in finding T_{h3} from T_{h2} is the initial density, ρ_{h1} , since the expansion of the hot side starts from the volume fraction η_1 . The final pressure, P_3 must be the same for both the hot and cool sides. The equations at State 3 are a function of only a single unknown, η_3 , so the problem is to find the root of the equation:

$$f(P) = P_{h3}(\eta_3) - P_{c3}(\eta_3) \quad (36)$$

This is readily done using the Brent root finding algorithm. That the problem always converges is illustrated in Figure 8 for the isobaric solution. That is, the pressure of the hot side decreases and the pressure of the cool side increases with increasing η_3 .

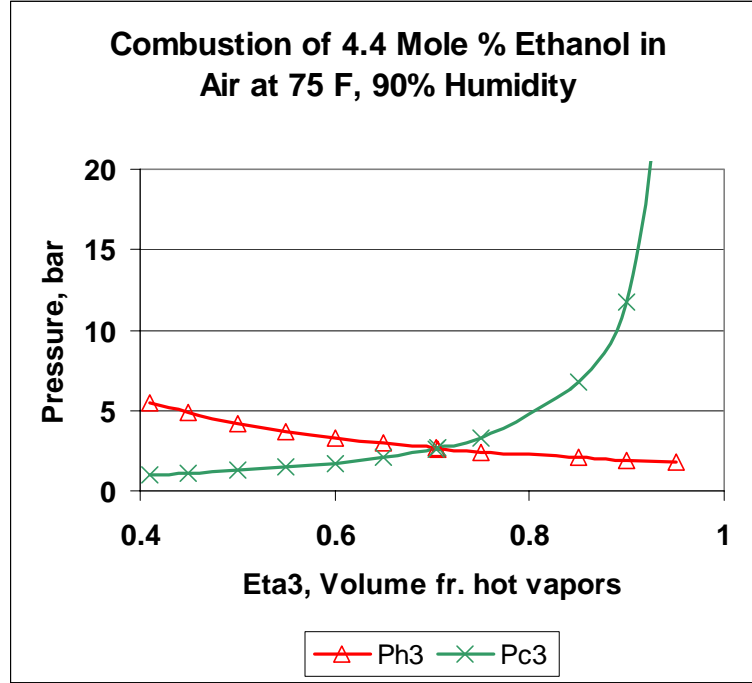


Figure 8 Example of Convergence of Pressure From Combustion in Room with Lean Ethanol Vapors in 41% of the Room Volume

The only difference between the two solutions is that for the isochoric solution, the intermediate pressure is taken from Eq. 33b. An analytic approximation for the isochoric solution is obtained from the expansion/compression formulas:

Compressed Conditions, State 3, Isobaric Solution

$$V_{h3} = V_{h1} \left(\frac{P_{h2}}{P_3} \right)^{1/\gamma_h} \quad (37a)$$

$$V_{c3} = (1 - V_{h1}) \left(\frac{P_1}{P_3} \right)^{1/\gamma_c} \quad (37b)$$

Adding the volumes and dividing by the total volume V gives:

$$1 = (1 - \eta_3) \left(\frac{P_1}{P_3} \right)^{1/\gamma_c} + \eta_3 \left(\frac{P_{h2}}{P_3} \right)^{1/\gamma_h} \quad (38)$$

If $\gamma_c = \gamma_h$ then Eq. 38 can be solved for P_3 in terms of η_3 :

$$P_3 = P_1 \left[\left(1 - \eta_3 \right) + \eta_3 \left(\frac{P_{h2}}{P_1} \right)^{1/\gamma} \right]^\gamma \quad (39)$$

Each assumed value of η_3 gives a value for the final pressure, P_3 . This pressure must give a density consistent with the initial mass in the room.

Example Pressure Calculations

Table 1 and Figure 9 show results from applying Eqs. 29-36 to an LFL concentration of ethanol in a room of volume 1800 m^3 . The important parameter values for this case are:

Flame Temp (K)	Mole Wt of Products	Hot Side γ	Cool Side γ	Conc (mole %)	Ambient Temp (K)
994	28.29	1.3562	1.3826	4.4	298

The isochoric solution gives temperatures that decrease below the flame temperature as the hot side expands, as should be the case. The isobaric solution gives hot side temperatures above the flame temperature, which is incorrect. The pressures predicted by the isobaric solution are considerably higher than those predicted by the isochoric. Even so, it has been found that for low values of the initial flammable volume fraction, η_1 , the isobaric solution is more accurate. At higher values of η_1 the isochoric solution is more accurate.

A comparison was made between experimental data and the pressures calculated with the isobaric solution in order to examine the level of conservatism associated with this solution. The experimental data are from the Bureau of Mines 12 foot diameter spherical explosion chamber⁸. The combustible gas mixture evaluated here was a $\text{CO-H}_2\text{-CH}_4\text{-CO}_2\text{-N}_2$ mixture occupying 25% of the chamber volume. The measured peak deflagration pressure was 32 psig. The calculated pressure for this case is approximately 35 psig. The calculated value is slightly higher than the experimental data, as would be expected.

Large overpressures, exceeding the strength of most room walls, windows, and explosion vent panels, occur with an initial flammable volume fraction in excess of 10% for both solutions. This illustrates the need for the next step in the process, calculating the pressures developed during the discharge of burned and unburned gases. This calculation is beyond the present scope.

Table 1 Example Calculations of Pressures From Partial Volume Combustion Before Vents Open

Initial η Vol % Fuel	Final η Vol % Burned	Max Pressure (psig)	Hot Side Temp (K)	Cool Side Temp (K)
5	11.3	1.5	743	316
10	21.2	3.0	760	324
20	37.7	6.1	793	339
40	61.6	12.6	852	366
5	14.9	2.4	1034	321
10	27.0	4.9	1072	334
20	45.3	10.2	1142	356
40	68.7	21.5	1259	395

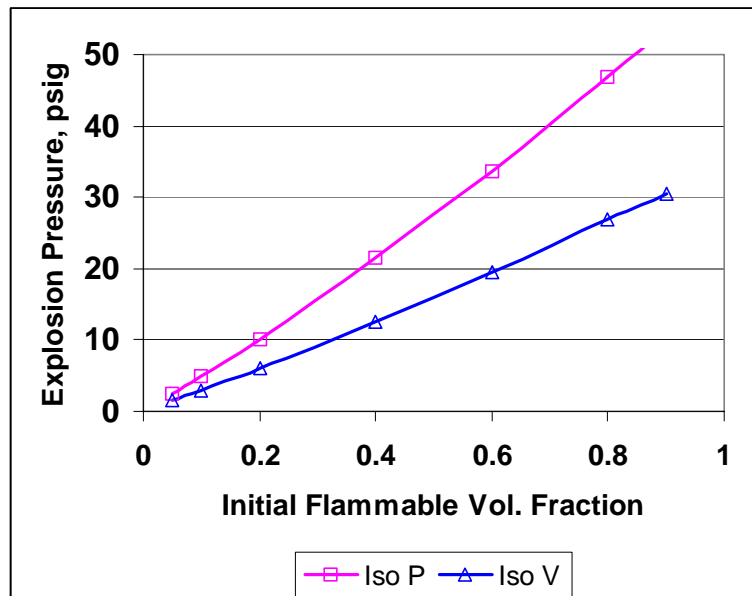


Figure 9 Comparison of Maximum Overpressure Predicted by Isochoric and Isobaric Models of Partial Volume Deflagration

Conclusions

A useful model is described for indoor concentration variation from an indoor leak or spill. The WELMIX model can be used as a design tool to evaluate mitigation strategies based on gas sensor systems. The model indicates the effect of varying ventilation rate, fresh air ratio, room size, and the effect of variables that influence the source rate such as pool diameter and floor drain placement. It can be used to estimate the maximum fraction of a room volume capable of containing a flammable mixture because of stratification or vertical concentration profiles. In this respect, it is useful for treating spill of moderately-volatile liquids like ethanol, ethylene oxide, and acetone.

The basic relationships for a general fire and explosion model are developed here and applied to calculate pressures built up in a partial volume deflagration before explosion vents open. Two alternative derivations are provided, isobaric and isochoric. For low fractions of the room volume with flammable vapors, the isobaric solution is found to better match a single experiment by the Bureau of Mines. The isobaric solution predicts higher explosion overpressures than the isochoric. These overpressures are found to be substantial, even when a relatively small volume fraction of a room contains flammable vapors. The relationships shown are building blocks for generalizing to a vented explosion model, but are fundamental and must hold true in any more general model.

Nomenclature For Indoor Dispersion

F_{ex} = mass rate exhausted from ventilation duct, kg/s

F_{sh} = mass rate of fresh air, kg/s

F_{in} = mass rate into room from ventilation duct, kg/s

F_{dis} = mass discharge rate into room, kg/s

F_{out} = mass rate leaving room, kg/s

M_i = molecular weight of component i, kg/kmole

M_{mix} = molecular weight of multicomponent mixture, kg/kmole

t = time, sec.

t_d = delay time in duct

V = room volume, m^3

w_c = mass fraction of contaminant component in the room

w_{cin} = mass fraction of contaminant component(s) in ventilation duct

w_{cdis} = mass fraction of contaminant component(s) from source

w_{chi} = mass fraction of contaminant at high alarm point

w_{clo} = mass fraction of contaminant at low alarm point

Nomenclature For Fire Model

a_f Air to fuel mass ratio, kg/kg

a_{fs} Stoichiometric air to fuel mass ratio, kg/kg

C_{pa} Heat capacity of moist air, J/(kgK)

C_p = Specific heat at constant pressure,

C_v = Specific heat at constant volume ($C_v = C_p - R$), and

f_{Rad} Fraction of energy of combustion radiated out fire plume

h_{fg} Heat of vaporization, J/kg

h_w = moles of water/mole of dry air

H_{comb} Heat of combustion, J/kg

H_i Specific enthalpy of component i , J/kg

g Gravitational constant, (9.81 m/s^2)

m_b Burn rate, kg fuel/s = $G_b A_{pool}$

m_{plume} Mass rate in fire plume, kg/s

P_a Atmospheric pressure, Pa

P_w Vapor pressure of water, Pa

R Universal gas constant.

H_{reac} Heat rate released by combustion, W

RH Relative humidity, fraction

T_a Ambient temperature, K

T_f Flame temperature, K

T_b Normal boiling point, K

y_w Mole ratio of water, mole/total moles

ρ_a Air density, kg/m^3

ρ_v Fuel vapor density, kg/m^3

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