The primary purpose of this paper is to examine the physical basis of the equations which govern enclosure fire behavior. A rigorous derivation will be presented for the conservation equations based on control volume principles and on the assumptions invoked in the "zone modeling" approach. Following those derivations, simple cases will be examined to display approximate mathematical solutions and their implications. Phenomena to be considered will include smoke filling of a compartment, the effect of thermal feedback on burning, and the production of combustion products in fuel-rich combustion conditions.

The results presented are not generally original, and are available in various sources. The value of this paper is to give the reader an opportunity to examine a logical development of the subject, and hopefully to learn about the behavior of enclosure fires through the approximate mathematical relationships given. These relationships are not intended as substitutes for complete computer fire models. They only serve to give approximate results, physical insight, and perhaps even guidance on achieving their solution by numerical means. In short, this presentation is offered as a tutorial on the subject of enclosure fire behavior using the zone modeling approach. In that regard, it assumes that the reader has a firm understanding of engineering fluid mechanisms and thermodynamics.

**CONTROL VOLUME EQUATIONS**

We start by developing the basic conservation laws for a moving control volume. The principles of a control volume analysis can be...
reviewed as necessary from texts on thermodynamics or fluid mechanics (for example, see S. Whitaker, *Introduction to Fluid Mechanics*, Prentice-Hall Inc., 1968). Since a control volume represents a specified region, the conservation equations in this form will be directly applicable to the appropriate "zones" or spatial regions of significance in enclosure fires.

Consider a reacting mixture of (perfect) gases in a specified volume Control Volume, shown below, which can move according to a selected surface velocity $w$.

![Control volume notation](image)

The velocity of species $i$ is

$$v_i = v + V_i \quad (1)$$

where $v$ is the bulk or mass weighted average velocity of the mixture with $N$ species:

$$v = \frac{1}{\rho} \sum_{i=1}^{N} V_i \rho_i \quad (2)$$

where $\rho_i$ is the density of species $i$ and

$$\rho = \sum_{i=1}^{N} \rho_i$$

is the mixture density \quad (3)

$$Y_i = \frac{\rho_i}{\rho}$$

is the mass fraction of species $i$ \quad (4)

$$X_i = \frac{M_i}{M} \quad Y_i$$

is the mole fraction of species $i$ \quad (5)

$M_i =$ molecular weight of species $i$ (e.g., g/g-mole)

$M =$ molecular weight of the mixture $= \frac{\sum (n_i M_i)}{\sum n_i}$ \quad where $n_i =$ number of moles of species $i$.

$\Sigma$ without limits implies $\sum_{i=1}^{N}$

$V_i$ is the diffusion velocity of species $i$, and is its velocity relative to the bulk flow, $v$.

By Fick's law:

$$\rho Y_i V_i = -\rho D_i \nabla Y_i$$

where $D_i$ is the diffusion coefficient of species $i$ in the mixture.

Overall Conservation of Mass

$$\frac{d}{dt} \iiint_{CV} \rho \, dV + \iiint_{GS} \rho \, (v - \mathbf{w}) \cdot ndS = 0 \quad (6)$$

Conservation of Mass for Species $i$

$$\frac{d}{dt} \iiint_{CV} \rho_i \, dV + \iiint_{GS} \rho_i \, (v + V_i - w) \cdot ndS$$

$$= \iiint_{CV} \dot{\omega}_i \, 'dV$$

where $\dot{\omega}_i$ is the production rate per unit volume of species $i$ due to chemical reaction.

It can be shown that by summing Equation 7 over all $N$ species, the left-hand side is identical to that of Equation 6. Hence,

$$\iiint_{CV} \sum_{i=1}^{N} \dot{\omega}_i \, 'dV = 0 \quad \text{or} \quad \sum_{i=1}^{N} \dot{\omega}_i = 0. \quad (8)$$

This demonstrates that mass is conserved in a chemical reaction.

Consider a simple complete chemical reaction in which a gaseous fuel ($F$) reacts with oxygen ($O$) and forms products ($P$). More than one product can be formed, but only one will be considered since generalizations to more products simply involve the particular stoichiometry relative to those particular species. For fire conditions, the stoichiometry of the particular reaction depends on the fuel, and on the relative amounts of air and fuel available. If sufficient air (in excess of that required by stoichiometry) is available, it is
reasonable to consider for a $\text{C}_x\text{H}_y\text{O}_z$ fuel that CO$_2$ and H$_2$O are the primary products of combustion. The production of CO, soot (smoke), H$_2$ and other species for compounds containing Cl, F, N, etc., are also possible. Some of these results can be estimated from the chemical formula of the fuel, but in general (especially for CO and smoke where no theoretical basis has been soundly established) empirical results from tests are needed. Two such devices are the "NBS Cone Calorimeter" and the "FMRC Flammability Apparatus". These test results are usually presented in terms of "yields" or the mass of species (or energy) produced per mass of fuel volatized or lost into the gas phase during thermal degradation — i.e., combustion or pyrolysis.

As a basis for developing the needed equations for room fire prediction, we will begin with an idealized stoichiometry for the reaction of a $\text{C}_x\text{H}_y\text{O}_z$ fuel with oxygen to be as follows:

$$\text{C}_x\text{H}_y\text{O}_z + \text{O}_2 \rightarrow \text{H}_2\text{O} + \text{CO}_2$$

or

$$r \text{ g Fuel (F)} + 1 \text{ g Oxygen (O)} \rightarrow (r+1) \text{ g Products (P)}$$

where the products here consist of a mixture of H$_2$O and CO$_2$ and are regarded as a single substance but could easily be treated separately according to their respective stoichiometries.

In general, the reaction (production) rate per unit volume for the fuel might be given as

$$\dot{w}_p^{(r+1)} = -k_F Y_F^P Y_O^m e^{-E/RT}$$

with $Y_F$ and $Y_O$ the respective fuel and oxygen mass fractions, $E$ the activation energy, $R$ the gas constant, $T$ the temperature, and $k_F$ a constant for the fuel. This equation describes Arrhenius kinetics for the fuel. Usually insufficient information is available, especially in a control volume approach, to utilize the relationship in Equation 10. However, knowing $\dot{w}_p^{(r+1)}$ allows one to determine the rates of the other species by Equation 9.

$$\dot{w}_o^{(r+1)} = \frac{1}{r} \dot{w}_p^{(r+1)}$$

(11a)

In enclosure fires and in many other practical forms of combustion, it is reasonable to assume that the rate of reaction is solely determined by the rate of fuel or oxygen supplied, i.e.,

$$\dot{w}_F = \int \int \int \dot{w}_F^{(r+1)} dV = \begin{cases} \text{fuel supply rate to CV} \quad \text{or} \\ \rho_r \text{ (oxygen supply rate to CV)} \end{cases}$$

whichever is smaller. This approach will be adopted. It leads to either leftover fuel or leftover oxygen in the exhaust flow stream.

Conservation of Energy for a Control Volume (for $N$ reacting species)

$$\frac{d}{dt} \int \int \int \sum_{i=1}^{N} \rho_i u_i dV +$$

(rate of change of internal energy)

$$\int \int \int \sum_{i=1}^{N} \rho_i h_i (v + V_i - \omega) \cdot n dS$$

(rate of net enthalpy flow rate out of CV)

$$= - \int \int \int p n \cdot \omega dS$$

(Pressure work term due to moving control volume)

$$- \int \int \int q'' n dS$$

(Rate of heat loss by radiation and conduction (convection) on the boundary of the CV)

$$+ \int \int \int \sum_{i=1}^{N} \tau_{ii} \cdot v_i dS$$

(Rate of work done by surface stresses $\tau_{ii}$ (excluding pressure) on the fluid in the CV)

$$+ \int \int \int \sum_{i=1}^{N} \rho_i f_i v_i dV$$

(Rate of work done by body forces per unit mass, $f_i$, on the fluid in the CV)

where $u_i$ is the internal energy per mass of species $i$, $h_i$ is the enthalpy per mass of species $i$

and

$$h_i = u_i + p_i / \rho_i$$

(14)
where \( p_i \) is the partial pressure of species \( i \),
where

\[
p = \sum_{i=1}^{N} p_i \text{ by Dalton's law for ideal gases. (15)}
\]

The enthalpy of each species is defined relative to a fixed standard reference state (25°C and 1 atm. pressure) i.e.,

\[
h_i = h_i^\circ + \int_{T_0}^{T} c_p \, dT \text{ for perfect gas} \quad (16a)
\]

and for constant specific heats

\[
h_i = h_i^\circ + c_p (T - T_0) \quad (16b)
\]

where \( T_0 = 25 \) °C and \( h_i^\circ \) is enthalpy of formation of the species \( i \) (and is usually taken as zero for elemental substances made of the same element as compared to compounds which can have positive or negative values for their enthalpies of formation).

For fire applications, the last two work terms in Equation 13 are considered negligible and will be dropped subsequently. Consider the LHS (left-hand-side) of Equation 13 and substitute

\[
\rho_i u_i = \rho_i h_i^\circ - p_i
\]

\[
h_i = h_i^\circ + c_p (T - T_0):
\]

and

\[
LHS = \frac{\partial}{\partial t} \iiint_{CV} \left( \sum_{i=1}^{N} \left( \rho_i h_i^\circ + \rho_i c_p (T - T_0) - p_i \right) \right) dV + \iiint_{GS} \sum_{i=1}^{N} \rho_i h_i^\circ (v + V_i - w) \cdot n \, dS \quad (17)
\]

Multiply Equation 7 by \( h_i^\circ \), since \( h_i^\circ \) is a constant it can be taken under the integral. Sum the resulting equation over \( i=1, N \) resulting in:

\[
\frac{\partial}{\partial t} \iiint_{CV} \sum_{i=1}^{N} \rho_i h_i^\circ \, dV + \iiint_{GS} \sum_{i=1}^{N} \rho_i h_i^\circ (v + V_i - w) \cdot n \, dS = 0
\]

Substitute Equations 17 and 18 into Equation 13 and use

\[
\sum_{i=1}^{N} \rho_i = \rho
\]

\[
\sum_{i=1}^{N} \rho_i c_p = \rho c_p
\]

where \( c_p \) is the specific heat of mixture (assumed constant).

\[
\frac{\partial}{\partial t} \iiint_{CV} (\rho c_p (T - T_0) - p) \, dV + \iiint_{GS} \sum_{i=1}^{N} \rho_i c_p (T - T_0) \, (v + V_i - w) \cdot n \, dS = -\iiint_{CV} \sum \dot{\omega}_i \, h_i^\circ \, dV - \iiint_{GS} p n \cdot w \, dS - \iiint_{GS} q'' \cdot n \, dS \quad (19)
\]

since \( c_p = \text{constant and } p = \rho RT \) for the mixture where \( R \) is the gas constant for the mixture which is assumed constant. Also

\[
c_v = c_p - R \text{ and } c_p/c_v = k \quad (20)
\]

By Equations 2 and 7 it can be shown that
Then Equation 19 becomes

\[
\frac{d}{dt} \int_V \rho c_p T_0 dV + \int_V \sum_{i=1}^N \rho c_{pi} T (v + V_i - \omega) \cdot n dS = 0.
\]

If \( c_{pi} \) is assumed identical for all species, from Equations 1 and 2 the last term is zero in Equation 22.

From the stoichiometry of Equation 11 it follows that

\[
- \sum_{i=1}^N \dot{\omega}_i h_i^s = - \left\{ \dot{\omega}_F h_F^s + \dot{\omega}_s h_s^s + \dot{\omega}_p h_p^s \right\}
\]

\[
= - \left\{ \dot{\omega}_F \Delta H \right\}
\]

where \(- \dot{\omega}_F \Delta H\) is the consumption rate of the fuel reacted and

\[
\Delta H = \sum_{i=1}^N \left\{ (\gamma_i h_i)_{\text{reactants}} - (\gamma_i h_i)_{\text{products}} \right\}
\]

where \( \gamma_i \) are the stoichiometric coefficients (mass basis) per unit mass of fuel reacted and \( \Delta H \) is the energy liberated per unit mass of fuel reacted in having the chemical reaction occur to completion with the initial and final states at \( T_0 \), the standard state. It should be noted the sign convention here is such that the heat of combustion is taken as positive. Alternatively, \( \Delta H \) is assigned to be negative in thermodynamics for an exothermic reaction in combustion. Note \( \dot{\omega}_F \Delta H \) is inherently negative since it was defined as a rate of production, and fuel is consumed (the negative of production). Thus \(- \dot{\omega}_F \Delta H\) is a positive energy release rate for an exothermic reaction.

The governing energy equation follows:

\[
\frac{d}{dt} \int_V \rho c_p T dV + \int_V \rho c_p T (v - w) \cdot n dS = - \int_{\text{CS}} pn \cdot w dS - \int_{\text{CS}} q'' \cdot n dS - \int_{\text{CS}} \sum_{i=1}^N \rho c_{pi} TV_i \cdot n dS
\]

\[
\int_{\text{CS}} [- \dot{\omega}_F] \Delta H \, dV - \int_{\text{CS}} pn \cdot w \, dS
\]

(heat loss)

The last term in Equation 22 has been dropped as an approximation in Equation 24. Also, it is a reasonable approximation to take \( c_p, c_v \) (R and \( k \)) to be properties of air since the mixture will contain a good deal of nitrogen from air in normal fire conditions.

The Equations 6, 7 and 24: mass, species and energy will be applied to control volumes appropriate to room fires. The entire region of the CV or distinct proportions will be considered to be homogeneous. Also the shapes will be taken as rectilinear, but could be generalized to arbitrary enclosure shapes.

**CONSERVATION LAWS FOR ENCLOSURE FIRES**

The choice of a control volume is based on the behavior observed for natural fires in enclosures. The behavior consists of the following:
the fire forms a buoyant plume which forms a layered and reasonably well-mixed upper and lower region of uniform temperature. These features are illustrated in Figure 1;

and shown to represent reasonably uniform temperature upper and lower gas and wall regions, at least at one measuring station in the enclosure in Figure 2. For a large space, the variations in temperature could be large due to heat loss. The flame plume region is distinct from these upper and lower regions and can be considered as a separate control volume.

The behavior described is valid provided that the momentum of the ceiling jet is low compared to the buoyancy of the jet. If the reverse were true, the system would be dominated by momentum, (as illustrated in Figure 3) and could result in a well-mixed region throughout the enclosure.

For the layered case, as shown in Figure 1, three gas-phase control volumes emerge:

1. upper hot layer,
2. lower cold layer,
and 3. fire plume - combusting region.

In developing the enclosure fire equations, it is assumed (sometimes implicitly) that the fire plume has negligible volume compared to the enclosure volume and can be considered as part of the upper layer control volume. This is an approximation and it should be noted that the extent of reaction (flame) is changing and may extend through the upper layer at some large fire conditions. Alternatively, two control volumes can be selected — one for the upper layer and one for the flame. The latter is useful when some average uniform flame plume properties are required, e.g., temperature, species, etc. In this choice, it may be useful to consider the flame plume as quasi-steady — neglecting type terms which suggest a small volume; whereas the upper layer is fully treated as unsteady. The first choice of considering one control volume for the flame and upper layer will be adopted as a start. This is shown in Figure 4, where \( CV_1 = \) upper layer + fire plume where the surface is selected as shown in Figure 4 such that \( w = 0 \) at the solid boundaries except at the lower face of the layer where \( w = v \), i.e., this layer's surface moves as the fluid that composes the stratified region conforms to it. Any fluid that enters \( CV_1 \) leaves due to pressure differences at openings, and due to shear mixing or buoyancy effects that destroy the stratified and

![Figure 1. Vertical Enclosure Fire Behavior](image1.png)

![Figure 2. Room temperatures with a wall vent at steady state](image2.png)

![Figure 3. Momentum controlled enclosure mixing (possible for high pressure combusting jet)](image3.png)
stable interface between the hot and cold layers. The cold region CV2 is the remainder of the enclosure gas volume. Some other assumptions follow:

1. No diffusion or conduction occurs at free boundary surfaces of the control volume.
2. Exchange of mass at free boundaries are due to bulk transport of fluid due to pressure or shear mixing.
3. Diffusion can occur at solid boundaries but is generally ignored.
4. The plume instantly arrives at the ceiling.
5. The mass or heat capacity of room contents is ignored compared to the enclosure structural wall, ceiling and floor elements.
6. The horizontal cross section of the enclosure is a constant area A.
7. The pressure in the enclosure is considered uniform in the energy equation, but hydrostatic variations account for pressure differences at free boundaries of the enclosure. \( p >> \rho gh \). In general the enclosure, \( p \), is much greater than the variations due to stable mixing.

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Figure 4. Control volumes selected in zone modeling

Figure 5. Types of flow exchange in room fires
to hydrostatics. For example, for \( p = 1 \text{ atm.} = 14.7 \text{ psi} = 10^2 \text{kPa} = 10^5 \text{ Pa} \), the hydrostatic variation for a height, \( H = 1 \text{ m} \), gives a pressure difference of \( \rho g H = 1.2 \text{ kg} \times 9.8 \text{ m/s}^2 \times 1 \text{ m} = 10 \text{ kg/m.s} = 10 \text{ N/m}^2 \).

8. Mass flow into the fire plume is due to turbulent entrainment, \( v_e \).

9. In the analysis to follow, we will consider the lower \( CV_2 \) to have properties equal to the surrounding fluid outside of the enclosure. This is not a necessary assumption, and it is straightforward to consider variable properties for the lower layer.

Flows through Openings –
Free Boundaries of \( CV \)

In most cases, flows across openings in fire conditions are due to pressure differences arising from temperature (density) differences or forced convection. In other cases, flows can arise due to mixing (shear or diffusion effects). The pressure differences can arise due to the fire itself or the ventilation system of the building. Some examples of possible flow exchange are given in Figure 5.

Flows due to pressure differences can be calculated by Bernoulli’s equation with a correction factor (generally known as an orifice flow coefficient as used in pipe flow analysis). The flow is shown in Figure 5A as a jet in the diagram below which can represent a horizontal or vertical cross section. The jet moving into the next space assumes the pressure of that space at some point in the jet where the cross-section of the jet is less than the cross-section of the opening. (This is known as the vena contracta in orifice flow and the flow coefficient accounts primarily for this decrease in cross-section.) On the streamline from 1 to 2, and assuming the velocity at 1 is negligible compared to the velocity at 2,

\[
v_2 = \sqrt{\frac{2(p_1 - p_2)}{\rho_1}}
\]  

(25)

where \( \rho_1 \) is the density of the fluid coming from space 1. The mass flow rate through the vent over its entire area is

\[
\dot{m} = C \int \int A \rho_1 v_2 \, dA
\]  

(26)

where \( A \) is the cross-sectional area of the vent and \( C \) is the flow coefficient (= 0.7). Typical profiles of velocity for pressure driven flows (Figures 5a & b) are given above.

For the natural convection case, we assumed that the pressure varies vertically in an enclosure only due to gravity, i.e., hydrostatics. Thus,
the jets associated with the vent flows in Figure 6a respond to the pressure on each side of the opening such that inside

\[ p = p(0) - \int_0^z \rho g dz \]  

(27a)

and

\[ p = p(0) - \int_0^z \rho g dz \]  

(27b)

outside the enclosure (in the "cold" environment) with properties denoted by \( (\cdot)_0 \). Note \( g \) is the acceleration due to gravity.

Hence, by Equation 25, the velocity at any height \( z \) in the jet is given as

\[ v(z) = \pm \sqrt{\frac{2(\Delta p)}{\rho}} \]  

(28a)

where \( \rho \) corresponds to the "in" or "out" flow according to where the flow originates, and

\[ \Delta p(z) = |(p - p_\infty)| \]  

(28b)

If the flow reverses direction as shown in Figure 6a, the point of change is called the neutral plane, \( N \), where \( \Delta p = 0 \) at \( z = N \). This is usually the case for most enclosure fire conditions with a wall vent.

The general calculation of vent flows requires knowledge of the pressure differences across each opening. For multiroom problems, this information comes from solving the governing conservation equations for each room. The vent mass flows will be a function of layer temperatures and room pressure. The room pressure is usually taken as the value at the floor and assumed uniform with height for Equation 24, but varies hydrostatically by Equation 27 in order to express the mass flow rates, Equation 26. These specific conservation equations will be presented shortly.

An illustration of flow modes due to natural convection arising from an enclosure fire is depicted below in Figure 7 as a fire grows to "fill" a room.

Here we have considered a uniform temperature external region with the same temperature as the cold lower region in the enclosure.

**Plume Entrainment**

Before considering the general conservation equations, we need to have an expression for the rate of flow into the fire plume over the height \( D \), to the interface. Many alternative expressions are available, but none are definitive nor can be derived from fundamental principles. They are all empirical. In general, the mass rate of entrainment, \( \dot{m}_e \), depends on the energy release rate of the fire, \( \dot{Q} \), the height, \( D \), and the geometry of the fire, \( G \) (e.g., pool fire, line fire, wall fire, chair fire, etc.)

\[ \dot{m}_e = \dot{m}_e(\dot{Q}, D, G) \]  

(29a)

For example, Zukoski\(^9\) gives for a point source axisymmetric plume of zero initial mass flow (at \( z = 0 \)):

\[ \dot{m}_e = \text{constant} \dot{Q}^{1.3} D^{5.0} \]  

(29b)

In Equation 29b, \( \dot{Q} \) is just the convected energy rate: the chemical energy release minus the energy radiated from the fire plume.

**Conservation of Mass**

Let us now consider Figure 4 and CV\(_1\). It is redrawn in Figure 8 with the flows indicated. With the assumptions previously given for the fluid in CV\(_1\) and CV\(_2\), and that all properties are uniform within these CV's (except when \( p \) is used to calculate mass flows); and Equation 6 is used to show

\[ A \frac{d}{dt} (p z) + \sum_{j \in \text{net out}} \dot{m}_j = 0 \]  

(30a)

where the second term represents the sum of the net mass flow rates out of the CV. For the mass flows in Figure 8

\[ A \frac{d}{dt} (p z) + \dot{m} - \dot{m}_e - \dot{m}_s = 0 \]  

(30b)
Figure 7a. Layer descending, cold flow leaves the vent

Figure 7b. Hot flow begins to leave the vent

Figure 7c. Layer interface below the vent and cold flow enters from the surroundings
Conservation of Species

Similarly, Equation 5 and Equation 7 can be used to derive the conservation of species $i$ for the CV1 in Figure 8.

\[ A \frac{d}{dt}(\rho z_i Y_i) + \sum_{\text{net out}} \dot{m}_j (Y_{ij} - Y_i) = \dot{\omega}_i \tag{31} \]

where $Y_{ij}$ is the value of the mass fraction of the $i$th species in the stream entering or leaving the CV (Note: for flows leaving, $Y_{ij} = Y_i$, the value in the CV) and $\dot{\omega}_i$ is the rate of production of $i$ in the CV.

If $[\dot{\omega}_F]$ is the rate of fuel reacted within CV1, then

\[ \dot{\omega}_b = \left( \frac{1}{r} \right) \dot{\omega}_F \quad \text{and} \quad \dot{\omega}_b = -\left( r + \frac{1}{r} \right) \dot{\omega}_F \]

by Equation 11 (for the stoichiometry considered). Then multiplying Equation 30a by $Y_i$ and subtracting it from Equation 31 yields:

\[ \rho z_i A \frac{dY_i}{dt} + \sum_{\text{net out}} \dot{m}_j (Y_{ij} - Y_i) = \dot{\omega}_i \tag{32a} \]

For the specific case of Figure 8, this becomes

\[ \rho z_i A \frac{dY_i}{dt} + \dot{m}_e (Y_i - Y_e) + \dot{m}_s (Y_i - Y_s) = \dot{\omega}_i \tag{32b} \]

Consider $i = F$ and $i = o$, and define a new vari-

\[ \beta = Y_F - rY_o \] so that Equation 32a becomes

\[ \rho z_i A \frac{d\beta}{dt} + \sum_{\text{net out}} \dot{m}_j (\beta_j - \beta) = 0 \tag{33} \]

For the specific case of Figure 8, let us consider that oxygen enters with the $\dot{m}_e$ stream at $Y_{oe}$, and is zero in the $\dot{m}_s$ stream. Then Equation 33 becomes

\[ \rho z_i A \frac{d\beta}{dt} + \dot{m}_e (\beta - \beta_e) - \dot{m}_s (\beta - \beta_s) = 0 \tag{34} \]

where

\[ \beta_e = r Y_{oe} (Y_{oe} = 0.233 \text{ in air}) \]

\[ \beta_s = Y_{ps} (= 1 \text{ if pure fuel}) \]

Furthermore, the energy release rate is assumed to be as follows:

\[ \dot{Q} = [-\dot{\omega}_F] \Delta H \tag{35a} \]

where

\[ [-\dot{\omega}_F] = \begin{cases} \dot{m}_s Y_F, & Y_o > 0 (or \text{ a critical}) \\ Y_o \text{ at extinction for} & \end{cases} \]

\[ r Y_o, \dot{m}_e, Y_o = 0 \tag{35b} \]

Equation 35b is an assumption based on the need to differentiate between fuel-controlled fires ($Y_o > 0$) and ventilation-limited fires ($Y_o = 0$); and the lack of any alternative model for $\dot{\omega}_F$ consistent with the "zone" model concept. Note by solving for $\beta$, one obtains $Y_o$ and $Y_F$ in the upper layer since when $Y_o = 0$, $Y_F > 0$ and when $Y_o > 0$, $Y_F = 0$ for the idealized stoichiometry given by Equation 9. Also it can be shown that

\[ \beta = Y_F + \left( \frac{r}{r+1} \right) Y_p \tag{36} \]

also satisfies Equation 34, so that $Y_p$ can instantly be found (and this can be generalized to many products - CO$_2$, H$_2$O, soot, ... provided the stoichiometry is known for the reaction).

Energy Equation

The energy equation for the CV1 in Figure 8 follows from Equation 24:

\[ \rho z_i A \frac{d\beta}{dt} + \sum_{\text{net out}} \dot{m}_j (\beta_j - \beta) = 0 \tag{33} \]
where $T_j$ is the temperature in the stream entering or leaving the CV, and $T$ is the temperature of the fluid within the CV.

Multiply Equation 30a by $c_p T$ and subtract from Equation 37

$$-A c_p T \frac{d}{dt} (p z_l) + p \frac{dz_l}{dt} A +$$

$$A c_v \frac{d}{dt} (p T z_l) + c_p \sum_{j \notin \text{out}} (T_j - T) \dot{m}_j$$

$$= \left[ -\dot{\omega}_F \right] \Delta H - \dot{Q}_{\text{net loss}}$$

Equation 40 is the most convenient form of the energy equation for the control volume used in enclosure fires. Note that the sum term is zero for all flows out of the control volume since $T_j = T$. Consequently it only contributes for inflows for which the sign of the mass inflow rates would be negative.

Ignoring the species equation for now, since it is independent of $p$ and $T$ and $z_l$, we have two equations for $p$, $T$ and $z_l$ given by Equation 30 and 40 where $p = p/RT$ is given by the Equation of State for an ideal gas. By applying the same equations to CV$_2$ - the lower layer we can find $T_e$ and since $p_e = p$ and $z_e = D = H - z_l$, we have two more equations. Thus, four equations (two energy and two mass), with four unknowns: $T$, $T_e$, $p$, $z_l$. As a first approximation, we could take $T_e = T_\infty$ the temperature of the surroundings. This assumption obviously eliminates $T_e$, and only three equations are needed. A useful form to these necessary equations is derived below by working with Equation 37. Since $p$ is considered uniform in the enclosure, we apply the energy equation to the entire fluid in the enclosure, CV $= CV_1 + CV_2$.

Apply Equation 37 to each region CV$_1$ and CV$_2$:

$$A c_v \frac{d}{dt} (p T z_l) + c_p \sum_{j \notin \text{out}} (T_j - T) \dot{m}_j$$

$$= \left[ -\dot{\omega}_F \right] \Delta H - \dot{Q}_{\text{net loss}}$$

It follows that

$$-A c_p T \frac{d}{dt} (p z_l) + A c_p \frac{d}{dt} (p T z_l)$$

$$-A z_l \frac{dp}{dt} + c_p \sum_j (T_j - T) \dot{m}_j$$

$$= \left[ -\dot{\omega}_F \right] \Delta H - \dot{Q}_{\text{net loss}}$$

or

$$A c_p \rho z_l \frac{dT}{dt} - A z_l \frac{dp}{dt} + c_p \sum_j (T_j - T) \dot{m}_j$$

$$= \left[ -\dot{\omega}_F \right] \Delta H - \dot{Q}_{\text{net loss}}$$

where the mass flow summation is only considered over the non-common boundary between the two CV's since these terms cancel at the common boundary.

For the specific case of Figure 8, Equation 40 gives

$$A c_p \rho z_l \frac{dT}{dt} - A z_l \frac{dp}{dt} + c_p \tilde{m}_e (T - T_e)$$

$$+ c_p \tilde{m}_s (T - T_s) = \left[ -\dot{\omega}_F \right] \Delta H - \dot{Q}_{\text{net loss}, CV_1}$$

(42)
and Equation 41 gives

\[
\frac{AH}{k-1} \frac{dp}{dt} + c_p T \frac{dn}{dt} + c_p \dot{m}_m T_e = \dot{Q}_a
\]

(43)

where \( \dot{m}_m \) is defined as an outflow from CV2 for this case. For the case of an ambient lower layer \( T_e = T \), the governing conservation equations are Equations 30, 42, and 43 for the unknowns \( p, T \) and \( z_l \). The mass flow rates all depend on these same variables, and once they have been determined the solution for particular species follows from solving Equation 32. Thus, these equations represent the conservation laws for the zone model formulation of enclosure fires. We shall now consider some special cases and approximate solutions.

**APPLICATIONS TO SPECIAL PHENOMENA**

We will now examine various stages for fire development. First, the phenomena of how smoke fills an enclosure during the initial stage of a fire will be examined. The pressures that result due to the fire energy release will be quantitatively analyzed to gain some insight into this process. Then we shall examine the characteristics involved in fire growth and the effect of enclosure conditions on fuel burning. Finally we shall examine the post flashover or fuel-rich fire case, and a proposal for computing the combustion products that result.

**Enclosure Pressures**

Consider the case of filling, i.e., Figure 7a where the descending layer is above the top of the opening. Consider \( mScpT_e \) small or lump it into the RHS (right-hand-side) of Equation 43 and call the RHS, \( Q_a \), the net energy added to the room gas. Also since \( \dot{m} = 0 \) as long as \( z > H_o \), we have

\[
AH \frac{c_p}{R} \frac{dp}{dt} + c_p m \dot{T}_e = \dot{Q}_a
\]

also

\[
T_e = T, \quad \frac{c_p}{R} = \frac{1}{k-1}, \quad c_p T_e
\]

\[
= \frac{cp}{\rho_m} (T_o \rho_e) = \frac{cp}{\rho_m} p = \frac{cp}{\rho_m (k-1)} p
\]

Hence,

\[
\frac{(AH)}{k-1} \frac{dp}{dt} + m \frac{\dot{m}}{\rho_m} \frac{(k-1)}{k} p = \dot{Q}_a
\]

(44)

By Equation 26 and 28

\[
\dot{m} = \rho A_o C \sqrt{\frac{2 (p - p_m)}{r_{oo}}}
\]

(45)

Let \( p - p_m \equiv \Delta p \) and substitute Equation 45 into Equation 44

\[
\frac{AH}{k-1} \frac{dp}{dt} + \dot{Q}_a \frac{k}{k-1} \frac{p}{\rho_m}
\]

\[
\sqrt{\frac{2}{r_{oo}} \Delta p} \frac{\Delta p (p - p_m)}{\rho_m} = \dot{Q}_a
\]

\[
\frac{AH}{k-1} \frac{dp^*}{dt} + \frac{C W_o H_o}{Q_o} \frac{k}{k-1} \frac{p^*}{\rho_m}
\]

\[
\sqrt{\frac{2}{r_{oo}} p^* \sqrt{p^{*}} (p^* + 1)} = 1
\]

where \( p^* = \Delta p/p_m \).

Let

\[
P = \frac{p^*}{\varepsilon^2}
\]

following from Baum and Rehm\(^8\)

\[
\tau = \frac{t(k-1)\dot{Q}_a}{\varepsilon^2 p_m (AH)}
\]

where \( AH = V \),

\[
\varepsilon = \frac{k}{k-1} \sqrt{\frac{p_m^2}{2 C W_o H_o}}
\]

or since \( a_w = \sqrt{k p_m \rho_m} = \sqrt{k R T_m} \)

is the speed of sound,

\[
\varepsilon = \frac{(k-1)}{\sqrt{2k} C W_o H_o} p_m a_w
\]

Hence

\[
\frac{dP}{d\tau} = 1 - \sqrt{P} (1 + \varepsilon^2 P)
\]

(46)

If there is no out flow, i.e. a sealed enclosure,

\[
\frac{dP}{d\tau} = 1 \text{ for } W_o H_o = 0
\]

Also at steady state \( \tau \rightarrow \infty \) and \( P = 1 \). For \( \varepsilon \) small, the solution is given as

\[
\tau = 2 \left[ \ln(1 - \sqrt{P})^{-1} - \sqrt{P} \right]
\]

(47)

This analysis follows that of Baum and Rehm\(^8\) and Zukoski\(^9\). Some results have been computed and
plotted in Figure 9.

\[ \tau = \frac{(k-1)\dot{Q}_a}{\varepsilon^2 p_{\infty} V} t \]

Figure 9. Pressure rise in enclosure due to sudden steady release of energy to the gas (\( Q_a \))

\[ \varepsilon = \frac{(k-1)\dot{Q}_a}{\sqrt{2k} \frac{w_o H_o P_o a_m} {p_{\infty} V}} \]

\[ \frac{(k-1)\dot{Q}_a}{p_{\infty} V} = \frac{100 kWh \times 10^3 J/s}{(0.7) (1m) (10^5 N/m^2) (341 m/s) H_o (m)} \]

\[ \varepsilon = \frac{10^3}{H_o (m)} \]

\[ \frac{(k-1)\dot{Q}_a}{p_{\infty} V} = \frac{(0.4) (100 kWh) \times 10^3}{(10^5 N/m^2) (40m^3)} = 10^{-2} s^{-1} \]

Consider the \( \Delta p \) rise at nearly steady state

i.e. \( P = 0.9 \) and \( \tau = 4.04 \)

Hence, we can find the pressure at 90% of steady state and the time to reach that value. The results are given below:

\[ \Delta p = \varepsilon^2 p_{\infty} P = 0.9 \left( \frac{10^{-3} N/m^2}{H_o^2} \right) \]

\[ \Delta p = \left( \frac{0.09}{H_o^2} \right) N/m^2 \]

\[ t = \varepsilon^2 \frac{V}{(k-1) \dot{Q}_a} \tau = \left( \frac{10^3}{H_o} \right)^2 (10^2) (4.04) \]

\[ t = 4.04 \times 10^{-4} \frac{s}{H_o^2} \]

It is seen from the above that the pressure rise is very low and its response is very fast. Hence the room pressure adjusts to changes in \( Q_a \) very

\( V = 40 m^3 \) for the volume,
\( Q_a = 100 kW \) for the net heat added to gas,
\( W_o = 1 m \) for the width of the vent,
and
\( H_o = 1, 0.1, 0.01 m \) and 0 closed for the height of the vent.

Let the flow coefficient \( C = 0.7 \)
\( p_{\infty} = 1 \) atm = 10^5 N/m^2

\( a_m \sqrt{k p_{\infty} / p_{\infty}} = \sqrt{\left( \frac{10^5 kg - m/s^2}{m^2} \right) / (1.2 kg/m^3)} = 341 m/s \)

From the solution to Equation 47

\[ \frac{\Delta p}{p_{\infty}} \leq \varepsilon^2 \]

since \( P \rightarrow 1 \) as \( \tau \rightarrow \infty \). The solution applies for vents below the smoke layer as shown in Figure 10. For the case of \( Q_a \) constant, if no vent is present and the enclosure is leak tight, the pressure continuously increases in time:

\[ P = \tau \]

Under these conditions the pressure will likely increase until the structure of the enclosure fails.

Let us consider an example:
quickly and \( \frac{dp}{dt} \) is likely to be nearly zero since the steady or quasi-steady value of \( p \) is likely to exist over time scales of most interest to fire behavior. But if the sealed case is considered for the same example with \( H_0 = 0 \),

\[
\Delta p = p_\infty \cdot \frac{(k-1) \dot{Q}_a t}{p_\infty V} = \frac{(k-1) \dot{Q}_a t}{V} \tag{50}
\]

For a 1 m² window, the \( \Delta p \) or \( H_0 = 0.01 \) m (or a 100 cm² hole) gives a force of 900 N or 200 lbs; while in a sealed system at 10s, the force is 2250 lbs. So even for an extremely small opening, roughly 3 ft. wide and 0.3 inches high, the force of 200 lbs is marginally on the brink of causing windows or other weak partitions to fail. On the other hand, a fire in a sealed space can very easily lead to high pressures and possible structural failure provided the fire is not first diminished by the depletion of available oxygen.

### Enclosure Smoke Filling.

In general Equations 43, 40 and 30a give sufficient information to solve for \( p \), \( T \), and \( z_l \) with appropriate relationships for the \( \dot{m}_j \) and heat losses to the boundary. This has resulted from the application of the energy equation to the upper and lower layers, and the mass conservation equation to the upper layer. Actually the temperature of the lower layer is not constant, but by assuming \( T_e = T_w \) we can apply the conservation of mass to the lower layer to obtain an alternative to Equation 30a. This is

\[
A \frac{d}{dt} (p \Delta) + \sum (\text{net out}) \dot{m}_j = 0 \tag{51a}
\]

For the CV₂ in Figure 11 we apply Equation 51a where \( \rho_e = \rho_\infty \) the value of the surroundings.

\[
\rho_\infty A \frac{d}{dt} (p \Delta) + \dot{m}_e (Q, \hat{D}, G) + \dot{m}_\infty (p, A_0) = 0 \tag{51b}
\]

where \( \dot{m}_e \) is the entrainment rate, Equation 29, and

### Table 1: Pressure Rise for a Room with Vent and Time at Nearly Steady State Due to a Constant Heat Release Rate

<table>
<thead>
<tr>
<th>( H_0 ) (m)</th>
<th>( \Delta p ) (N/m² or Pa)</th>
<th>( t ) (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.09 ( (1.3 \times 10^{-5}) )</td>
<td>4.10 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>0.1</td>
<td>9. ( (1.3 \times 10^{-3}) )</td>
<td>4 ( \times 10^{-2} )</td>
</tr>
<tr>
<td>0.01</td>
<td>900. ( (1.3 \times 10^{-1}) )</td>
<td>4 ( \times 10^{-1} )</td>
</tr>
</tbody>
</table>

Since \( \Delta p = p_\infty e^2 \) in the steady limit and approaches it rapidly, from Equation 46 and its definitions:

\[
\dot{m}_\infty = \rho_\infty A_0 C \sqrt{\frac{2}{\rho_\infty} \frac{(k-1)}{k}} \sqrt{\frac{2}{RT_e}} \frac{\dot{Q}_a}{CWH_0 p_\infty} = \frac{\rho_\infty}{\rho_\infty} \left( \frac{(k-1)}{k} \right) \frac{\dot{Q}_a}{RT_e} \tag{52}
\]

For \( \dot{Q}_a \) small (or for a vent in the hot layer – see Zukowski) we can ignore \( \dot{m}_\infty \) and by using Equation 29b

\[
\dot{m}_e = C_1 \dot{Q}_a^{\frac{13}{3}} D^{\frac{53}{3}} \tag{53a}
\]

\[
\frac{dD}{dt} = \frac{C_1 \dot{Q}_a^{\frac{13}{3}}}{\rho_\infty A} D^{\frac{53}{3}} \tag{53a}
\]

\[
-\frac{3}{2} \int_H^D \hat{D} (D^{-2/3}) = -\int_0^t \frac{C_1 \dot{Q}_a^{\frac{13}{3}}}{\rho_\infty A} dt
\]

\[
-D^{-2/3} + H^{-2/3} = \frac{2 C_1 \dot{Q}_a^{\frac{13}{3}}}{3 \rho_\infty A} t \tag{53b}
\]

\[
D = \left[ 1 + \frac{2 C_1 H^{2/3} \dot{Q}_a^{\frac{13}{3}}}{3 \rho_\infty A} t \right]^{-32}
\]
This gives an approximate relationship for the layer height as it descends. Note that as $D$ becomes smaller, the rate of descent decreases by Equation 53a. As the layer descends past the vent top as indicated by Figure 7c, Equation 53b is no longer valid. Its application beyond that point would overestimate the layer’s descent since mass loss from the layer is not accounted for. At some distance below the top of the vent, $D$ is likely to equilibrate for a steady fire, and the application of Equation 53b to that point should give a reasonable estimation.

**Upper Layer Temperature**

Consider the energy equation for the upper layer as Equation 42, where we take $dp/dt = 0$ as an approximation so that

$$p = p_\infty$$

and $\rho_\infty T_\infty = \rho T$;

therefore

$$A_p \rho_\infty T_\infty z_l \frac{1}{T} \frac{dT}{dt} + c_p m_\varepsilon (T - T_\infty) + c_p m_\varepsilon (T - T_s) = [- \omega_p] \Delta H - \dot{Q}_{\text{net, loss}}$$

(54)

If $D$ is approximately stationary, then flow into the fire plume is constant by Equation 29b. Also by conservation of mass in the lower layer,

$$\dot{m}_e = \dot{m}_{\text{in, vent}}$$

or by conservation of mass in the upper layer,

$$\dot{m}_e = \dot{m}_{\text{out, vent}} - \dot{m}_s$$

By considering the $\Delta p$ that arises in Figure 7c, these vent flows can be determined from $T$, $D$ and $N$. We have not developed this result explicitly here. Let it suffice to say that

$$\dot{m}_{\text{out, vent}} = \dot{m}_{\text{in, vent}} = C A_p \sqrt{H_0} f(T)$$

where $f(T)$ is a known function of $T$. It can be shown that the behavior with $T$ is not strongly dependent on temperature for $T > 200$ °C as sketched in Figure 12.

For a constant vent flow, $z_l = H - D$ constant, and $\dot{m}_e$ negligible compared to $\dot{m}_e = \dot{m}_\text{vent}$ an approximate solution can be determined from Equation 54 for $T$ as a function of $t$. By linearizing Equation 54, it can be shown that unless $Q$ is rapidly changing, $T$ will not change rapidly with time. Let us therefore consider solutions where $dT/dt = 0$, i.e. steady or quasi-steady points.

### Equation 54

$$\dot{m}_e = \dot{m}_{\text{in, vent}}$$

**The Rate of Energy Release, $R^*$**

$$R^* = [- \omega_p] \dot{H}$$

(56)

Consider the nature of these terms.

#### The Rate of Energy Release, $R^*$

$$R^* = \begin{cases} m_s \Delta H, Y_o > 0 \\ \rho Y_o e \dot{m}_\varepsilon \Delta H, Y_o = 0 \end{cases}$$

(56)

from Equation 35b. Also in a fire, because the surroundings get hot, $m_s$ will respond to external heating as well as to heating from its own flame. Hence

$$m_s = m_{s_0} + \Delta m_s$$

(57)

where $m_{s_0}$ is due to flame heating and

$$\Delta m_s = q_{\text{external}}/L$$

where $L$ is the heat of gasification and $q_{\text{external}}$ is the heat transfer rate from the enclosure. Since $q_{\text{external}}$ depends nonlinearly on $T$ because of predominant radiant heating, $m_s$ increases sharply as $T$ increases. Once $Y_o$ becomes 0 in the layer, we expect $m_s$ to increase slightly if $m_\varepsilon$ and $T$ increases (Figure 12).

### The Loss, $L^*$

$$L^* = \dot{Q}_{\text{net, loss}} + c_p m_\varepsilon (T - T_\infty)$$

(58)

Since $\dot{Q}_{\text{net, loss}}$ depends on heat transfer through and to the enclosure structure, we see that $L^*$ is a linear...
function of $T$ as a first approximation, and increases more strongly as $T$ increases due to radiation heat transfer. The behavior of $R^*$ and $L^*$ are sketched in Figure 13 with $T$. The three intersections $s_1$, $s_2$, $s_3$ are all solutions to Equation 55 but only $s_1$ and $s_3$ are stable. The characteristics of these stable solutions are given as follows:

$s_1$
- little thermal feedback to fuel
- excess air available
- pre-flashover

$s_3$
- strong thermal feedback
- excess fuel ($Y_o = 0$)
- incomplete combustion (CO)
- post-flashover

Generally $s_1$ is a fuel-controlled fire, burning like a free burn fire and $s_3$ is a ventilation-controlled fire. As $L^*$ decreases due to more heat loss to the enclosure surfaces, a point of tangency between the $R^*$ and $L^*$ curves is possible. This tangency yields a possible "jump" condition that is suggestive of the onset of "flashover." Thomas et al.\textsuperscript{11} discuss these possibilities and their cause more completely. Although a true "jump" discontinuity only applies to this steady-state analysis, its occurrence signifies large changes in certain variables over small changes in time. These effects would be manifested in a more complete solution to the transient problem. Moreover these "jumps" dramatize the physical significance of such events as flashover or extinguishment in enclosure fires.

**Post-flashover and Ventilation-limited Fires**

Once the state of the fire is at $s_3$ it does not have sufficient oxygen supplied to burn all of the fuel. The fire is fuel-rich and the combustion is incomplete meaning that the idealized reaction assumed in Equation 9 is not valid. For our hydrocarbon fuel, the "fuel-rich" combustion products will include, in addition to $H_2O$ and $CO_2$, $CO$ and $H_2$ and other hydrocarbons. Also the oxygen may remain in the products. At the current time, there is no practical way to predict this system of combustion products in state $s_3$. But studies by Zukoski\textsuperscript{12} and Beyler\textsuperscript{13} have shown that, for a wide range of fuel and air flow conditions under steady-state, the species concentrations could be correlated by a single flow variable. The flow variable is the equivalence ratio, $\phi$, defined in terms of the flow streams into the control volume composed of the fire plume and upper layer. It is defined as follows:

$$\phi = m_o/r m_e X_o,e$$

where $r$ is the stoichiometric fuel to oxygen mass ratio for the idealized reaction completely going to $CO_2$ and $H_2O$. Correlations have shown that the actual species concentrations for a given fuel could be represented solely as:

$$Y_i = Y_i(\phi) \quad (59)$$

A typical plot is sketched in Figure 14 for some of the species. The nature of the excess fuel may contain many hydrocarbon species due to pyrolysis of the primary fuel. At $\phi = 1$, the idealized reaction would have $Y_o = 0$ and $Y_F = 0$ marking the boundary of the fuel-lean and rich regimes. This idealized model was the basis for the energy release relationship assumed in Equation 56. Such an idealization does not allow us to estimate CO, but could be used to give a rough approximation of the major species ($O_2$, $CO_2$, $H_2O$) at least up to $\phi = 1$. Beyler\textsuperscript{13} shows the extent to which these estimations are accurate.
The correlations given by Equation 59 have been shown valid only under steady-state conditions. Therefore it is not obvious how this concept should be extended to unsteady conditions, or when the fuel source is totally within the upper layer so that \( \dot{m}_u = 0 \), or \( \phi \) is undefined. Since the need to estimate hazardous conditions to humans requires the prediction of CO and \( O_2 \), and it is known that the production rate of CO can increase by at least an order of magnitude between \( \phi < 1 \) and \( \phi > 1 \), a prescription for computing CO concentrations after flashover in the ventilation-limited fire state is essential. A proposed analysis is considered below. It has not been verified, but is worth presenting in the context of this tutorial on enclosure fires to show the application of control volume analysis and a potential to expand the applicability of zone modeling.

Consider the control volumes in Figure 15 which now explicitly distinguishes between the flame or reacting zone (CV2) and the rest of the upper layer gases (CV1). The flows are shown as before (i.e. Figure 8) except \( \dot{m}_f \) is the entrained flow rate into the flame from the upper layer gases. The concentrations in the flame are designated by the subscript \( R \) while the species in the upper layer have no additional subscript. By appropriately applying Equation 32a to each of the control volumes, it follows that CV1:

\[
m_1 \frac{dY_i}{dt} - \dot{m}_R (Y_{i,R} - Y_i) = 0 \tag{60}
\]

and for CV2:

\[
m_2 \frac{dY_{i,R}}{dt} - \dot{m}_s (Y_{i,s} - Y_{i,R}) - \dot{m}_t (Y_i - Y_{i,R}) = \dot{w}_i \tag{61}
\]

where \( m_1 \) and \( m_2 \) are the masses in CV1 and CV2 respectively, \( Y_{i,s} \) is the mass fraction of \( i \) in the fuel stream, and \( Y_{i,e} \) is the mass fraction of \( i \) in the oxidizer stream.

From Equation 60 we see that under steady conditions, \( Y_{i,R} = Y_i \), so that we expect the concentrations in the reaction zone to follow the correlations given by Equation 59. Now introduce \( \beta \) as in Equation 33, i.e. \( \beta = Y_F - rY_o \) where \( F \) designates fuel and \( o \) designates oxygen, and \( r \) is the idealized stoichiometric ratio. We seek to compute the mixture fraction \( Z \), for which the chemical production rates are defined in terms of the idealized reaction. Thus,

\[
\dot{w}_i = \dot{w}_i \frac{rY_o}{r} \tag{11a}
\]

as in Equation 11a. The mixture fraction is defined for the flame (CV2) as

\[
Z_R = \frac{\beta_R - \beta}{\beta - \beta} \tag{62a}
\]

and for the upper layer (CV1) as

\[
Z = \frac{\beta - \beta}{\beta - \beta} \tag{62b}
\]

Letting \( i = o \) and \( F \) in Equations 60 and 61 and then subtracting to eliminate \( \dot{w}_i \), allows one to generate corresponding equations in \( Z \) and \( Z_R \). It will be assumed that there is only fuel in the fuel stream, and \( Y_{o,e} \) is a constant in the oxidizer stream. Thus, \( \beta_s = 1 \) and \( \beta_e = -rY_{o,e} \).

Hence,

\[
Z_R = \frac{Y_{RF} + r(Y_{o,e} - Y_{R,o})}{1 + rY_{o,e}} \tag{63a}
\]

\[
Z = \frac{Y_{F} + r(Y_{o,e} - Y_o)}{1 + rY_{o,e}} \tag{63b}
\]

The equations for \( Z \) and \( Z_R \) became

\[
m_1 \frac{dZ}{dt} + \dot{m}_R (Z - Z_R) = 0 \tag{64a}
\]

and

\[
m_2 \frac{dZ_R}{dt} + \dot{m}_s (Z_R - 1) + \dot{m}_t (Z_R - Z) = 0 \tag{64b}
\]

Note under steady state conditions, it can be shown from Equations 64a and 64b that

\[
Z = Z_R = \frac{1}{1 + \frac{1}{rY_{o,e} \phi}} \tag{65}
\]
Thus, at the steady state there is a one-to-one corres-
pondence between $\phi$ and $Z$ and $Z_R$ for a given fuel.
This suggests that the correlations of Beyler and
Zukowski could have been expressed alternatively
in terms of $Z$ or $Z_R$. The significance of $Z$ (or $Z_R$) is
that for the state of oxygen equal to the supply con-
centration $Y_{o,e}$, $Z = 0$ ($\phi = 0$); and for the state of
pure fuel, $Z = 1$ ($\phi \to \infty$).

The following hypothesis is put forth as a means for
utilizing the data correlations in the form given by
Equation 59 in the context of an unsteady enclosure
fire analysis. It is assumed that the fire source is
the key element since that is where all of the reac-
tions take place. It is also assumed that $Z_R$ is
the primary variable (analogous to $\phi$ in the steady-
state) that determines the extent of the reaction
and its products. Thus, it is assumed that the ana-
logue to Equation 59 is

$$Y_{i,R} = Y_{i,R} (Z_R)$$

(66)

where this equation is determined from the data
correlations of Equation 59 for which $Y_i = Y_{i,R}$ and
$Z_R$ is given by Equation 65. Thus $Y_{i,R}$ can be deter-
mined from data of the form of Figure 14, and $Y_i$ for
the upper layer can be determined from Equation
60. The critical step in this analysis, however, is to
determine the extent of the reaction zone, CV$_2$. This
is needed in order to compute $m_2$, $m_e$ and $m_R$. So
some further assumptions will be necessary to
implement this analysis. All of this is needed to get
a key variable: the CO produced in the post-
flashover fires.

One difficulty with the above analysis is that it
requires a knowledge of the extent of the reaction
zone in order to estimate $m_R$. This is not easily
done. A way to avoid this difficulty is to consider the
flame and upper layer control volumes of Figure 15
as one homogeneous region as was previously done
in deriving the layer conservation equations. Again
the underlying hypothesis is a generalization of
Equation 66 which says that the mass fraction, $Y_i$, at a region or location association with a turbulent
fire is a unique function of the mixture fraction, $Z$,
at that same location. Let us now alternatively
develop an equation for $Z$ in this newly defined CV
—all of Figure 15.

With $m$ the total mass in CV$_1 + CV_2$, the conserva-
tion of mass is

$$\frac{dm}{dt} + \dot{m} - \dot{m}_e - \dot{m}_s = 0$$

(67)

The conservation of species using Equation 32a is
for oxygen,

$$m \frac{dY_o}{dt} + (\dot{m}_e + \dot{m}_s) Y_o - \dot{m}_e Y_{o,e} = \dot{\omega}_o$$

(68a)

and for the fuel,

$$m \frac{dY_F}{dt} + (\dot{m}_e + \dot{m}_s) Y_F - \dot{m}_s = \dot{\omega}_F = r\dot{\omega}_o$$

(68b)

By multiplying Equation 68a by $-r$ and adding it to
Equation 68b, we can have an equation for $Z$, the
mixture fraction (Equation 62b) for the CV$_1 + CV_2$
homogeneous region. It can be shown that

$$\frac{m \, dZ}{dt} + (1 + Y_{o,e} r \phi) Z + Y_{o,e} r \phi$$

(69)

For steady state conditions this equation obeys
Equation 65 as in the other analysis. But here no
explicit solution for $m_R$ is needed. Indeed, current
steady-state data for specific fuels from Beyler and
Zukowski give us the quantitative relationships for
the $Y_i$ in terms of $\phi$ or $Z$. Thus, in a gen-
eral compartment fire analysis we need to only solve
Equation 69 along with the other conservation
equations to obtain $Z$ for the problem of interest.
Once done, the data-correlations give us the layer
concentrations, e.g. CO, O$_2$, H$_2$ etc. Note that if the
lower layer $Y_{o,e}$ is not constant, the preceding anal-
ysis must be modified, but the same procedure
should apply provided the hypothesis of Equation
59 is valid. Recent work by Zukoski and co-workers
presented at the Second Symposium on Fire Safety
Science, Tokyo, June, 1988 demonstrates that
transient results can be correlated with the steady
results of Equation 59. This is very satisfying and
e encouraging.

**CONCLUDING REMARKS**

This analysis has been presented to help describe
the basic principles and assumptions used in model-
ing enclosure fires. It is intended as a tutorial to
aid in the understanding of the enclosure fires. The
basic conservation laws were presented for reacting
systems and applied specifically to the zone model-
ing description of enclosure fires -- homogeneous upper and lower gas regions. Useful forms of the conservation of mass, Equation 30; the conservation of species, Equation 32; the conservation of energy, Equation 40 or its one of its alternatives for the entire enclosure gas, Equation 43, were derived for the zone model system. Some basic principles on vent flows were presented, but the details of mass and heat exchange phenomena have been left for the reader to pursue elsewhere. As the equations were developed, attempts were made to formulate approximate solutions for special cases so that one might develop some physical insight and quantitative assessments. Such insight is not always possible when viewing the results of the more complete computer solutions. The analyses presented here are in no way substitutes for more exact computer results, but serve to enhance our understanding and the interpretation of results to more complex problems.

REFERENCES


Nomenclature

A area

$\rho$ specific heat at constant pressure

cv specific heat at constant volume

$D_i$ diffusion coefficient

D layer position

E activation energy

f body force per unit mass

g gravitational acceleration

G geometric variables

h enthalpy per unit mass
$h_i$ enthalpy of formation of species $i$

$H$ height

$H_o$ height of soffit above floor

$k$ specific heat ratio, $c_p/c_v$

$L$ heat of gasification

$L^*$ heat loss rate, Equation 58

$m$ mass

$M_i$ molecular weight of species $i$

$M$ molecular weight of mixture

$n$ unit normal vector

$n_i$ moles of species $i$

$N$ height of neutral plane above floor

$p$ pressure

$p^* = ((p - p_o)/p_o$)

$P$ $p^*/\varepsilon^2$

$p_i$ partial pressure of species $i$

$q$ heat flow

$Q$ energy release

$r$ stoichiometric ratio of mass of fuel to mass of oxygen

$R$ gas constant

$R^*$ energy gain rate, Equation 56

$S$ surface area

$t$ time

$T$ temperature

$u$ internal energy per unit mass

$v$ bulk velocity

$V_i$ species velocity

$V$ volume

$w$ control volume velocity

$W$ width

$X_i$ mole fraction of species $i$

$Y_i$ species mass fraction

$z$ height from floor

$z_l$ layer height

$Z$ mixture fraction, Equation 63

$\beta$ conserved variable, Equation 33

$\varepsilon$ dimensionless variable, Equation 46

$\gamma$ stoichiometric coefficients

$\Delta H$ heat of combustion (positive for exothermic)

$\phi$ equivalence ratio, Equation 59

$\rho$ bulk density

$\rho_i$ species density

$\omega_i$ mass production of $i$ due to chemical reaction

$\tau$ dimensionless time, Equation 46

**Subscripts**

$a$ added

$i$ species

$F$ fuel

$o$ oxygen

$P$ products

$\infty, o, r$ reference state

$e$ entrained flow

$l$ upper layer

$s$ fuel flow stream

$1, 2$ upper, lower layer respectively

**Superscripts**

($) per unit time

($) per unit area

($) per unit volume

($) reference state