AN EMPIRICAL MODEL OF THE YIELD OF CARBON MONOXIDE IN FIRES

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ABSTRACT

Carbon monoxide (CO) is considered to be the most important toxic gases that may be contained in fire effluents. Hence, it will be very beneficial for the evaluation of the hazard of smoke if the prediction of CO can be successfully introduced into fire models.

Several experiments conducted to date suggest that the yield of CO is strongly affected by 'equivalence ratio'. So it seems worthwhile to develop an empirical model of CO yield as a function of equivalence ratio based on the existing experimental data, and to use this model as the source term in fire models for the prediction of CO concentrations in the buildings.

In this paper, we introduce a combustion model of propane and determine each parameter used in the model as a function of equivalence ratio. The species assumed to be generated in the model are CO₂, CO, O₂, H₂O, H₂, C and unburned fuel. The model agrees reasonably well with the results of the existing experiments.

Keywords: carbon monoxide, chemical species, equivalence ratio, propane, fire model, smoke

1. INTRODUCTION

1.1 Background of the study

It is generally recognized that smoke is the major cause of deaths in building fires. To date restricting the use of combustible materials and installing smoke control systems have been the primary measures to cope with the smoke hazards.

However, a rational approach to fire safety should include adequate evaluation of the actual level of smoke hazard since fire safety measures may accompany increase of construction costs and inconvenience to building users.

With the progress in fire modeling in recent years[1,2], we are beginning to obtain reasonable means to predict the thermal environment

caused by building fires. However, the prediction of the toxic environment remains virtually unchallenged.

Of the toxic gases that can be contained in smoke, carbon monoxide (CO) is considered to be the most important. Accordingly, efforts to comprehensively evaluate the hazards of smoke would benefit if CO prediction could be introduced successfully into fire models.

1.2 Existing studies

(1) Experimental studies

The typical configuration of fire in a building space may be illustrated as Fig. 1. The space are often assumed to be stratified into two layers: an upper layer filled with

Figure 1. Schematic of Species Yield Tests

hot vitiated smoky gases and a lower layer colder and less vitiated. Also the setups of the existing experiments for investigating the issue of CO yield may realize similar condition.

Several experiments have been conducted to date using steady state fire [3]:

Beyler [4] and Zukoski et al. [5, 6] conducted several experiments using a pool or burner fire source. The burning rates range over 10–200kW, and the air supply rates were controlled by adjusting the height between the fire source surface and the interface of the two layers. A “catch food” was installed above the fire source to capture combustion products. (The catch food was about 1m square.) The temperature and the concentrations of CO, CO₂, O₂ and other species of the smoke layer were measured. Experiments were carried out for various fuels, burning rates and fresh air supply rates.

Beyler used several types of hydrocarbon as fuel and concluded that the yield of carbon monoxide is much larger under fuel-rich condition than fuel-lean condition. Yields of the major species were well correlated to equivalence ratio, although depended on the chemical structure of the fuel.

Zukoski et al. carried out experiments using natural gas, ethylene and propylene as the fuels, and correlated each species yield as a function of equivalence ratio. They also set up an apparatus that allowed fresh air to be injected into the upper layer to simulate

an unsteady state scenario such as the transient development of the upper layer in the early stage of room fires. They concluded that the species yield is primarily a function of the upper layer’s equivalence ratio, and is not dependent on that of the plume flow entering the upper layer. They found that, when the layer temperature is above about 700K, species yield depends on temperature.

Kim et al. [7] carried out experiments using methanol pool as the fire source and a 30cm cubic enclosure with various size of openings. They proposed a method for estimating species yields based on measured O₂, CO₂ and CO, although they did not refer to unburned fuel and soot.

Tewarson [8] used “Quartz tube” instead of a stratified two-layer system, and concluded that the yield of CO depends weakly on the scale of turbulent fires, but strongly on the chemical structure of the materials and the rate of ventilation.

(2) Studies with Numerical Analyses

Several studies with numerical analyses have also been conducted.

Nakaya [9] proposed a simple model for predicting concentrations of O₂, CO₂, CO as combustion products. In his model, the ratios of fuel vapor and air are assumed, but the decomposition process of the fuel and its properties must be given as input data.

Cooper [10] attempted to develop a model for predicting the species yield in two layer fire based on the layer equivalence ratio concept, which would take into account the oxygen in the layer as well as the oxygen supplied through fire plume and doorway flow, but the methodology seems too complicated to be incorporated into multiple room fire models.

1.3 Purpose of the study

The principal difficulty in predicting the concentration of CO in building spaces lies in that we know very little about the actual

mechanism for CO yield in fire.

However as described previously, many experiments suggest that CO yield is strongly affected by equivalence ratio, i.e., it becomes significant when the air supply is small, but negligible when the air supply is sufficient.

It, therefore, seems appropriate to develop an empirical model that determines CO yield as a function of equivalence ratio based on the existing experimental data, and then use this model as the source term for two layer fire models to predict CO concentrations in building fires.

In this paper, we describe a theoretical model for species yield developed for propane fuel based on this thought, for the first step of this study. The reasons for development of theoretical model are follows:

(1) Conservation of chemical species

Direct use of the numerical values obtained from experiments might seem possible to predict chemical species yields in fire environment. But experimental data may contain measurement errors which may produce theoretical contradictions if used in a two-layer zone model, because conservation of chemical species could not be assured. A theoretical model is necessary to ensure the conservation of chemical species.

(2) Establish of correlation between equivalence ratio and species concentrations

Two layer zone models generally involve unsteady state prediction, which makes calculation of equivalence ratios very complicated. On the other hand, an algorithm is already available to predict concentrations of each species, if the rates of species yields are given. It is therefore more convenient to establish a correlation between equivalence ratio and species concentrations because this allows equivalence ratios to be calculated.

(3) Modeling of theoretical combustion process

Most experiments only used such fuels as hydrocarbon and alcohol. Therefore, a theoretical combustion model is needed to

predict for other types of fuels which were not experimented or which are difficult to test, such as solid fuel.

2. METHODOLOGY OF THIS STUDY

For the first step, a combustion process and chemical species yield are modeled, and the parameters of this model are defined to well fit the existing experimental data. We begin with modeling propane fire because existing experimental data are most available for this fuel.

The influence of layer temperature on species yields has been reported [6], but is ignored in this paper.

3. SPECIES YIELD MODEL

3.1 Equivalence ratio

We assume that air is composed solely of O_2 and N_2 , ignoring the other chemical species due to their relatively small fractions. Fuel is assumed to be composed of carbon, hydrogen, oxygen and nitrogen. The chemical equation of a complete combustion can be expressed as:

The rates of yield of species in this reaction can be expressed as:

$$W_\ell = \frac{(\nu''_\ell - \nu'_\ell) M_\ell}{\nu'_f M_f} m_b \quad (2)$$

Using Eq. (2), stoichiometric fuel/air ratio Φ_s becomes as follows:

$$\begin{aligned} \Phi_s \equiv \frac{W_f}{W_a} &= \frac{-m_f}{-\frac{1}{Y_{O_2}^a} \cdot \frac{\nu'_{O_2} M_{O_2}}{\nu'_f M_f} m_f} \\ &= Y_{O_2}^a \left(\frac{\nu'_f M_f}{\nu'_{O_2} M_{O_2}} \right) \end{aligned} \quad (3)$$

On the other hand, the fuel/air ratio of combustion under an arbitrary condition Φ_a is defined as:

$$\Phi_a = \frac{m_f}{m_a} \quad (4)$$

Finally, the equivalence ratio, in other words, normalized fuel/air ratio Φ becomes as follows:

$$\Phi \equiv \frac{\Phi_a}{\Phi_s} = \frac{\frac{m_f}{m_a}}{Y_{O_2}^a \left(\frac{\nu'_f M_f}{\nu'_{O_2} M_{O_2}} \right)} \quad (5)$$

3.2 Burning rate of fuel

It is assumed that the burning rate of propane is determined by the smaller of the fuel inputs and the fuel that can be burned by the available air. More specifically, the burning rate m_b is given as follows:

a) when $\Phi \leq 1$ (fuel lean case)

$$m_b = m_f \quad (6.1)$$

b) when $\Phi > 1$ (fuel rich case)

$$m_b = \frac{\nu'_f M_f}{\nu'_{O_2} M_{O_2}} m_{O_2} = Y_{O_2}^a \left(\frac{\nu'_f M_f}{\nu'_{O_2} M_{O_2}} \right) m_a \quad (6.2)$$

3.3 Assumptions for a combustion model of propane fires

(1) Products of combustion

The model of the combustion and the products is illustrated in Fig. 2. The assumptions are made as follows:

- Of the fuel that burns, portion r undergoes complete combustion and yields CO_2 and H_2O .
- Of the remaining portion: $1-r$, portion s yields hydrocarbon, possibly propane fuel itself.
- The remainder: $(1-r)(1-s)$ undergoes incomplete combustion and portion p_1 , p_2 and q_1 yields CO , C and H_2 , respectively. It yields possibly CO_2 and H_2O as well.

(2) Chemical equation of the combustion model

Using the same symbols for the portion of the yield of each product as in Fig. 2, the combustion model is expressed in a chemical formula as follows. Here hydrocarbon is assumed as the same as C_3H_8 for simplicity.

If the combustion is complete the value of the parameters become: $r = 1$, $s = p_1 = p_2 = q_1 = 0$, respectively. When the com-

Figure 2. Combustion Model of Propane

bustion is incomplete, these values are different and change depending on the degree of incompleteness of the combustion. The intention of this study is to find the values for the parameters which give acceptable agreement with the existing experimental data.

3.4 Yield of Species

(1) Rates of yield of Species

Based on the combustion model described above, the rates of yield of the species are given as follows:

a) when $\Phi \leq 1$ (fuel lean case)

Applying Eq. (2) to the chemical Eq. (7), and noting Eq. (6.1), we obtain the rates of yield of the species as:

$$\begin{aligned} W_f &= -\{1-(1-r)s\}m_f \\ W_{O_2} &= -\left[5r + (1-r)\left(1-s\right)\left\{5 - \left(\frac{3}{2}p_1 + 3p_2 + 2q_1\right)\right\}\right]M_{O_2} \\ &\quad - \frac{M_f}{M_f} m_f \\ W_{CO_2} &= \frac{3\{r + (1-r)(1-s)(1-p_1 - p_2)\} M_{CO_2}}{M_f} m_f \\ W_{CO} &= \frac{3(1-r)(1-s)p_1 M_{CO}}{M_f} m_f \\ W_C &= \frac{3(1-r)(1-s)p_2 M_C}{M_f} m_f \\ W_{H_2O} &= \frac{4\{r + (1-r)(1-s)(1-q_1)\} M_{H_2O}}{M_f} m_f \\ W_{H_2} &= \frac{4(1-r)(1-s)q_1 M_{H_2}}{M_f} m_f \end{aligned} \quad (8.1)$$

b) when $\Phi > 1$ (fuel rich case)

Using Eq. (2), Eq. (7) and Eq. (6.2), we obtain:

$$\begin{aligned} W_f &= -\frac{\{1-(1-r)s\}M_f}{5 M_{O_2}} Y_{O_2}^a m_a \\ W_{O_2} &= -[r + (1-r)(1-s) \\ &\quad \left\{1 - \frac{1}{5}\left(\frac{3}{2}p_1 + 3p_2 + 2q_1\right)\right\}] Y_{O_2}^a m_a \end{aligned}$$

$$\begin{aligned} W_{CO_2} &= \frac{3\{r + (1-r)(1-s)(1-p_1 - p_2)\} M_{CO_2}}{5 M_{O_2}} \cdot Y_{O_2}^a m_a \\ W_{CO} &= \frac{3(1-r)(1-s)p_1 M_{CO}}{5 M_{O_2}} Y_{O_2}^a m_a \\ W_C &= \frac{3(1-r)(1-s)p_2 M_C}{5 M_{O_2}} Y_{O_2}^a m_a \\ W_{H_2O} &= \frac{4\{r + (1-r)(1-s)(1-q_1)\} M_{H_2O}}{5 M_{O_2}} \cdot Y_{O_2}^a m_a \\ W_{H_2} &= \frac{4(1-r)(1-s)q_1 M_{H_2}}{5 M_{O_2}} Y_{O_2}^a m_a \end{aligned} \quad (8.1)$$

(2) Normalized yield of Species

Normalized yield of species is defined as the ratio of the actual yield to the maximum possible theoretical yield. The maximum possible theoretical yield of each species W^* is given as follows:

$$\begin{aligned} W_f^* &= -m_f, \quad W_{O_2}^* = -\frac{5 M_{O_2}}{M_f} m_f, \\ W_{CO_2}^* &= \frac{3 M_{CO_2}}{M_f} m_f, \quad W_{CO}^* = \frac{3 M_{CO}}{M_f} m_f, \\ W_C^* &= \frac{3 M_C}{M_f} m_f, \quad W_{H_2O}^* = \frac{4 M_{H_2O}}{M_f} m_f, \\ \text{and } W_{H_2}^* &= \frac{4 M_{H_2}}{M_f} m_f \end{aligned} \quad (9)$$

In general, the normalized yield of a species $\bar{W}$ is given by dividing the yield rate of the species in Eq. (8.1) and Eq. (8.2) by the corresponding value in Eq. (9), however, here we use a special definition for fuel for convenience of comparing with Beyler's data [4], i.e.:

$$\bar{W}_f = 1 - \frac{W_f}{W_f^*} \quad (10)$$

Thus, $\bar{W}$ for each species becomes as follows:

a) when $\Phi \leq 1$ (fuel lean case)

$$\begin{aligned} \bar{W}_f &= (1-r)s \\ \bar{W}_{O_2} &= r + (1-r)(1-s) \\ &\quad \left\{1 - \frac{1}{5}\left(\frac{3}{2}p_1 + 3p_2 + 2q_1\right)\right\} \end{aligned}$$

$$\begin{aligned}
\bar{W}_{\text{CO}_2} &= r + (1-r)(1-s)(1-p_1-p_2) \\
\bar{W}_{\text{CO}} &= (1-r)(1-s)p_1 \\
\bar{W}_{\text{C}} &= (1-r)(1-s)p_2 \\
\bar{W}_{\text{H}_2\text{O}} &= r + (1-r)(1-s)(1-q_1) \\
\bar{W}_{\text{H}_2} &= (1-r)(1-s)q_1
\end{aligned} \quad (11.1)$$

b) when $\Phi > 1$ (fuel rich case)

$$\begin{aligned}
\bar{W}_f &= 1 - \{1 - (1-r)s\} / \Phi \\
\bar{W}_{\text{O}_2} &= [r + (1-r)(1-s) \\
&\quad \left\{1 - \frac{1}{5} \left(\frac{3}{2} p_1 + 3p_2 + 2q_1 \right) \right\}] / \Phi \\
\bar{W}_{\text{CO}_2} &= \{r + (1-r)(1-s)(1-p_1-p_2)\} / \Phi \\
\bar{W}_{\text{CO}} &= (1-r)(1-s)p_1 / \Phi \\
\bar{W}_{\text{C}} &= (1-r)(1-s)p_2 / \Phi \\
\bar{W}_{\text{H}_2\text{O}} &= \{r + (1-r)(1-s)(1-q_1)\} / \Phi \\
\bar{W}_{\text{H}_2} &= (1-r)(1-s)q_1 / \Phi
\end{aligned} \quad (11.2)$$

Where use was made of the definition described by Eq. (5) as well as Eq. (8), Eq. (9) and Eq. (10).

3.5 Species concentrations in Gas layer

A typical configuration of fire in a space is illustrated in Fig. 1. Also, the setups of the existing experiments to investigate the issue of CO yield may be reduced to similar configuration.

In such a case, the concentration of species in the layer has one-to-one correspondence to equivalence ratio. This correlation is expressed as follows.

(1) Conservation for the Gas layer

Considering the overall mass and species concentration for steady state, we obtain the following equations:

1) Overall mass balance

$$m_e = m_f + m_a \quad (12)$$

2) Species balance

$$Y_\ell m_e = Y_\ell^f m_f + Y_\ell^a m_a + W_\ell \quad (13)$$

From Eq.(12) and Eq.(13), the mass fraction of species ℓ in the layer Y_ℓ becomes

$$\begin{aligned}
Y_\ell &= \frac{m_f}{m_a + m_f} Y_\ell^f \\
&\quad + \frac{m_a}{m_a + m_f} Y_\ell^a + \frac{1}{m_a + m_f} W_\ell
\end{aligned}$$

Using the fuel/air ratios defined by Eq. (3), Eq. (4) and Eq. (5), this becomes:

$$\begin{aligned}
Y_\ell &= \frac{\Phi_a}{1 + \Phi_a} Y_\ell^f + \frac{1}{1 + \Phi_a} Y_\ell^a \\
&\quad + \frac{1}{m_a + m_f} W_\ell \\
&= \frac{\Phi_s \Phi}{1 + \Phi_s \Phi} Y_\ell^f \\
&\quad + \frac{1}{1 + \Phi_s \Phi} Y_\ell^a + \frac{1}{m_a + m_f} W_\ell \quad (14)
\end{aligned}$$

(2) Concentration of each Species in the layer

Substituting W_ℓ in Eq. (8.1) and Eq. (8.2) into Eq. (14) yields the mass fraction of species ℓ in the layer. The mass fraction of each species becomes:

a) when $\Phi \leq 1$ (fuel lean case)

$$\begin{aligned}
Y_f &= \frac{(1-r)s\Phi_s\Phi}{1 + \Phi_s\Phi} \\
Y_{\text{O}_2} &= \frac{1 - \left[r + (1-r) \left\{ 1 - s \left\{ 1 - \frac{1}{5} \left(\frac{3}{2} p_1 + 3p_2 + 2q_1 \right) \right\} \right\} \right]}{1 + \Phi_s\Phi} Y_{\text{O}_2}^a \\
Y_{\text{CO}_2} &= \frac{\Phi_s\Phi}{1 + \Phi_s\Phi} \cdot \frac{3\{r + (1-r)(1-s)(1-p_1-p_2)\} M_{\text{CO}_2}}{M_f} \\
Y_{\text{CO}} &= \frac{\Phi_s\Phi}{1 + \Phi_s\Phi} \cdot \frac{3(1-r)(1-s)p_1 M_{\text{CO}}}{M_f} \\
Y_{\text{C}} &= \frac{\Phi_s\Phi}{1 + \Phi_s\Phi} \cdot \frac{3(1-r)(1-s)p_2 M_{\text{C}}}{M_f} \\
Y_{\text{H}_2\text{O}} &= \frac{\Phi_s\Phi}{1 + \Phi_s\Phi} \cdot \frac{4\{r + (1-r)(1-s)(1-q_1)\} M_{\text{H}_2\text{O}}}{M_f} \\
Y_{\text{H}_2} &= \frac{\Phi_s\Phi}{1 + \Phi_s\Phi} \cdot \frac{4(1-r)(1-s)q_1 M_{\text{H}_2}}{M_f} \quad (15.1)
\end{aligned}$$

b) when $\Phi > 1$ (fuel rich case)

$$\begin{aligned}
 Y_f &= \frac{[\Phi - \{1 - (1-r)s\}] \Phi_s}{1 + \Phi_s \Phi} \\
 Y_{O_2} &= \frac{\left(1-r\right) \left[1 - (1-s) \left\{1 - \frac{1}{5} \left(\frac{3}{2} p_1 + 3p_2 + 2q_1\right)\right\}\right]}{1 + \Phi_s \Phi} \\
 Y_{O_2}^a & \\
 Y_{CO_2} &= \frac{Y_{O_2}^a}{1 + \Phi_s \Phi} \cdot \frac{3\{r + (1-r)(1-s)(1-p_1 - p_2)\} M_{CO_2}}{5 M_{O_2}} \\
 Y_{CO} &= \frac{Y_{O_2}^a}{1 + \Phi_s \Phi} \cdot \frac{3(1-r)(1-s)p_1 M_{CO}}{5 M_{O_2}} \\
 Y_C &= \frac{Y_{O_2}^a}{1 + \Phi_s \Phi} \cdot \frac{3(1-r)(1-s)p_2 M_C}{5 M_{O_2}} \\
 Y_{H_2O} &= \frac{Y_{O_2}^a}{1 + \Phi_s \Phi} \cdot \frac{4\{r + (1-r)(1-s)(1-p_1)\} M_{H_2O}}{5 M_{O_2}} \\
 Y_{H_2} &= \frac{Y_{O_2}^a}{1 + \Phi_s \Phi} \cdot \frac{4(1-r)(1-s)q_1 M_{H_2}}{5 M_{O_2}} \quad (15.2)
 \end{aligned}$$

Incidentally, the volume fraction of each species can be obtained by multiplying the mass fraction in Eq. (15.1) and (15.2) by the ratio of the average molecular weight of air to the molecular weight of the species (carbon (C) is the only exception). That is:

$$X_\ell = Y_\ell \left(\frac{M_a}{M_\ell} \right) \quad (16)$$

4. DETERMINATION OF THE PARAMETERS

Here we attempt to determine the values of the parameters introduced into the combustion model so that the model agrees reasonably well with the results of existing experiments on CO yield.

4.1 In the case of complete combustion

The layer mass fraction, volume fraction and the normalized yield of species for complete combustion as a fraction of equivalence ratio Φ are given in Figs. 3 (a), (b) and (c), respectively. They are obtained by setting the parameters in Eq. (11) and Eq. (15) to $r = 1$, $s = p_1 = p_2 = q_1 = 0$, respectively.

4.2 In the case of including incomplete combustion

Perfectly efficient combustion cannot be expected in an uncontrolled combustion system such as a fire.

Beyler's results [4] of the experiments for propane fire are shown in Figs. 5 and 6. We observe that the approximate tendencies of fuel, CO_2 , H_2O , and O_2 agree with those with Fig. 3, both in the layer volume fractions and the normalized yields. However, the data for CO and H_2 reveal that these species start to be produced from about 0.6 and 0.8, respectively, which implies that the combustion begins to be incomplete from about $\Phi = 0.6$.

Figure 3. Calculated Results of Species Yield in the case of Complete Combustion

Figure 4. Calculated Results of Species Yield in the case of including Incomplete Combustion

Figure 5. Comparisons of Volume Fraction between Experimental Data⁴⁾ and Predicted Results for Propane

So, we introduced the following model in order to take into account the influence of incomplete combustion.

(1) when $\Phi \leq 1$ (fuel lean case)

From Fig. 5 (b), we notice that the volume fraction of CO and H_2 becomes larger as the value of Φ increases. Therefore, the portion of complete combustion should decrease as the value of Φ increases. Let r_0 be the fraction of air that is used effectively to produce the normal products, i.e. CO_2 and H_2O , when $\Phi = 1$. In other words, $r = r_0$

when $\Phi = 1$. Then, it will not be so inadequate to assume that

$$r = 1 - (1 - r_0)^{(1/\Phi)^n} \quad (17)$$

Note that $1/\Phi$ represents the normalized air/fuel ratio. The r might be interpreted as the probability with which fuel will react with oxygen when there is excess air. Although we do not know the order of reaction, $n = 2$ gives an acceptable result as far as empirical curvefitting is concerned.

After several trials, the following values

Figure 6. Comparisons of Normalized Yield between Experimental Data⁴⁾ and Predicted Results for Propane

have been found to give a reasonable agreement with Beyler's data:

$$\begin{aligned} r &= 1 - (1 - r_0)^{(1/\Phi)^2}, \quad r_0 = 0.75 \\ s &= 0.4 \\ p_1 &= 0.6 \\ p_2 &= 0.1 \\ q_1 &= 0.25 \end{aligned} \quad (18.1)$$

(2) When $\Phi > 1$ (fuel rich case)

For $\Phi > 1$, we are unable to obtain satisfactory agreement between the predict-

ed result and existing experimental data by changing the value of r only. So, we assume that the rate of complete combustion is constant, and that the yields of CO and H₂ increase as the rate of air supply relative to fuel decreases, in other words, p_1 and q_1 increase with the value of Φ .

Since this reduces the yield of CO₂ and H₂O produced from the part of incomplete combustion in the model shown in Fig.2. and accordingly, the consumption of O₂ as well,

the remained O_2 increases, though slightly.

So, in order to avoid this tendency, we assume that the rate of unburned fuels, s , decreases as the value of Φ increases.

As the result of several trials, it is found that the following values give a reasonable agreement with the experimental data:

$$\begin{aligned} r &= 0.75 \\ s &= 1 - (1 - s_0)^{(1/\Phi)^2}, s_0 = 0.4 \\ p_1 &= p_{10} \times \Phi^{1/2}, p_{10} = 0.6 \\ p_2 &= 0.1 \\ q_1 &= q_{10} \times \Phi^{1/2}, p_{10} = 0.25 \end{aligned} \quad (18.2)$$

4.3 Comparison between predicted results and Beyler's data

The calculated results of the upper layer volume fractions and the normalized yields of the species are shown in Fig. 4.

The results in Fig. 4 are compared with Beyler's data in Fig. 5 (a) for the volume fractions of CO_2 , H_2O and O_2 and in Fig. 5 (b) for CO , H_2 and unburned fuel, respectively. Beyler estimated unburned fuel volume fraction on the basis of CH_2 , but in our model is assumed as C_3H_8 . So, In Fig. 5 (b), recalculated unburned fuel on CH_2 basis is also shown.

Fig. 6 (a)~(f) shows the normalized yield of the various species compared to Beyler's experimental data.

While the general agreement in Fig. 5 and Fig. 6 is reasonable, some differences are still noticed. For example, in Fig. 5 (a), the calculated volume fraction of O_2 is higher, and that of H_2O is lower than the corresponding data from Beyler's experiments. However, we notice that Beyler's data for the normalized yields of O_2 and H_2O are sometimes larger than the maximum possible theoretical value, so apparently a certain degree of error is involved in the measurements. Therefore the differences in the volume fractions of O_2 and H_2O between the calculated and the real values may be smaller than shown in Fig. 5.

In Fig. 6 (e), the tendency of the yield of H_2 is different for $\Phi > 1$, but we have not been

able to obtain very successful agreement.

As for soot (C), there is no data available to make comparison because of the difficulties of measurement.

5. CONCLUDING REMARKS

In this paper, we introduced a combustion model for propane and determined each parameter used in the model as a function of equivalence ratio by using existing experimental data. The model agrees reasonably well with the results of existing experiments. We believe that its accuracy is sufficient for the purpose of using it in two layer zone models. We will try to extend the model to accommodate more generic fuels, and to incorporate it into a two layer zone model for predicting species yields and concentrations in transient fires.

SYMBOLS

m_b	mass burning rate of fuel (kg/s)
m_ℓ	mass rate of species ℓ (kg/s)
M_ℓ	molecular weight of species ℓ (kg/mol)
$\overline{W}_\ell$	rate of yield of species ℓ (kg/s)
$\overline{W}_\ell$	normalized rate of yield of species ℓ
X_ℓ	volume fraction of species ℓ in the layer (m^3/m^3)
$Y_\ell^f, Y_\ell^a, Y_\ell$	mass fraction of species ℓ in fuel, air and in the layer, respectively (kg/kg)
$Y_{O_2}^a$	mass fraction of oxygen in the air (kg/kg)
ν'_ℓ	stoichiometric coefficient of the species ℓ in reactant system
ν''_ℓ	stoichiometric coefficient of the species ℓ in product system
Φ	Equivalence Ratio, Normalized fuel/air ratio
Φ_s	stoichiometric fuel/air ratio

SUBSCRIPTS

F,f	fuel
a	air
e	exhaust
ℓ	chemical species

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