PREDICTION OF FLAME RADIATION AND TEMPERATURE IN POLYMER COMBUSTION

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ABSTRACT

The influence of fire ventilation on flame radiation is important in compartment fires especially for under-ventilated combustions. An approximate model for predicting flame radiant power and mean flame radiative temperature for both well- and under-ventilated polymer fires is proposed on the basis of $r$-correlations, in which the role of flame sootiness as well as the effect of fire ventilation is considered. The results were calculated for several typical polymers, and the effects of fire ventilation, chemical composition and structure of fuels, soot particle concentration and fire size were also investigated. The comparison with experimental data and the prediction from the Global Flame Radiation Model of de Ris and Orloff has been found to be satisfactory. This study attempts to provide: (1) a deeper scientific understanding of the effect of fire ventilation on flame radiation, and (2) available correlations, for the analysis of compartment fires.

Key words: Flame Radiation, Flame Temperature, Fire Ventilation, Polymer.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>area of compartment opening (m$^2$)</td>
</tr>
<tr>
<td>$A_f$</td>
<td>flame area (m$^2$)</td>
</tr>
<tr>
<td>$A_v$</td>
<td>burning area of fuel (m$^2$)</td>
</tr>
<tr>
<td>$C$</td>
<td>enclosure constant (kg / sm$^{5/2}$)</td>
</tr>
<tr>
<td>$C_0$</td>
<td>constant between 2 and 6</td>
</tr>
<tr>
<td>$C_2$</td>
<td>Planck's second constant</td>
</tr>
<tr>
<td>$D$</td>
<td>diameter of fuel bed (m)</td>
</tr>
<tr>
<td>$E$</td>
<td>entrainment coefficient</td>
</tr>
<tr>
<td>$f_v$</td>
<td>soot volume fraction</td>
</tr>
<tr>
<td>$H$</td>
<td>height of compartment opening (m)</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>general correlation coefficient</td>
</tr>
<tr>
<td>$\beta$</td>
<td>shift correlation coefficient</td>
</tr>
<tr>
<td>$r$</td>
<td>ventilation-controlled combustion parameter</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>flame emissivity</td>
</tr>
<tr>
<td>$\eta_s$</td>
<td>generation efficiency of soot</td>
</tr>
<tr>
<td>$\xi$</td>
<td>slope correlation coefficient</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>density of soot particles (kg / m$^3$)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stefan–Boltzmann constant</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>equivalence ratio</td>
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</table>
As a basic mechanism of heat transfer, flame radiation is very important in many combustion problems. It becomes the dominant mode of heat transfer in fires as the fuel bed diameter increases beyond about 0.3 m, and determines the growth and spread of fires in compartment.

With a few exceptions (e.g. methanol and paraformaldehyde), most liquid and solid fuels burn with luminous diffusion flames, as a result of the effect of emission from minute carbonaceous particles of diameters of the order of 10⁻¹⁻¹⁰₀ nm. While within a flame, these soot particles attain high temperatures and each one acts as a minute black or grey body. It is well known that emission from the soot particles is much larger than emission from the molecular emitters, such as H₂O and CO₂. Generally speaking, the "sootier" the flame, the lower its average temperature. It was found that the non-luminous methanol flame has an average temperature of 1200°C, while the luminous flames of kerosene and benzene were much cooler, 990°C and 921°C respectively. Thus, to a great extent, flame radiation and temperature depends on the flame sootiness because of the heat loss mechanism.

The Global Flame Radiation Model was recently presented by de Ris and Orloff[2] on the basis of smoke-point principle, which can be used to predict the flame radiant fraction and global flame temperature for fuels burning in air. It was found to be an excellent predictor of flame radiation for many common fuels for well-ventilated combustion.

During compartment fires, air supply is limited, fire ventilation is one of the main determinants of fire processes in many cases.[3][4] In their early stages, compartment
fires are well–ventilated, and easy to control and extinguish. However, if they are allowed to grow with limited ventilation and large fuel surface area, flashover is created, and the fires become under–ventilated. At this stage, heat release and soot formation are governed to a great extent by fire ventilation. Theoretically, with decrease in ventilation, the combustion efficiency decreases, whereas the concentration of soot particles increases. Despite its importance, the effect of ventilation on flame radiation and temperature for under–ventilated fires have been often assumed or omitted in many combustion analyses due to a lack of available correlations and scientific understanding.

In this study, an approximate model for predicting flame radiant fraction and mean flame radiative temperature was established, the calculations were performed by using this model and Global Flame Radiation Model for six typical polymers involving in both the small–scale and the large–scale fires, and the effects of ventilation, chemical composition and structure of fuels, soot concentration and fire scale were examined for both well– and under–ventilated combustion. The goal of this study is to provide a simple model for prediction of flame radiation and temperature, and a deeper scientific understanding of the effects of fire ventilation on polymer fire behavior, for compartment fire analyses.

**MODEL FORMULATION**

If a flame is assumed to be a homogeneous soot–gas volume with well–distributed temperature $T_f$, according to the Stefan–Boltzmann equation, the total radiant power from the flame is proportional to $T_f^4$, i.e.

$$Q_R = A_f \rho \sigma (T_f^4 - T_\infty^4)$$ (1)

1. Equivalence ratio

The fire ventilation is expressed most commonly in terms of mass fuel–to–air or mass fuel–to–oxygen stoichiometric ratio:[5]

$$\Phi = \frac{k_s \dot{m}}{Em_{air}}$$ (2)

where $E$ is the entrainment coefficient, and is estimated to be about 0.8 in the calculation of $\Phi$. When $\Phi < 1.0$, fires are defined as well–ventilated fires, and when $\Phi > 1.0$, fires are defined as under–ventilated fires. A correlation for the inlet air flow rate during a compartment fire, through an opening, was first formulated by Kawagoe[6]:

$$\dot{m}_{air} = CA\sqrt{H}$$ (3)
where the value of enclosure constant C ranges from 0.40 to 0.61 kg/s m^2, depending on the flow coefficient of the opening. The commonly used value is 0.52 kg/s m^2.

2. Flame size and shape
For simplicity, flame shape is approximated to a cylinder for natural diffusion flames. The flame height is given by

\[ L_f = a\dot{Q}_A^{2/5} - bD \]  

in the range of \( 7 < \dot{Q}_A^{2/5} / D < 700 \, \text{kW}^2 / \text{m} \), where the coefficients \( a = 0.23 \), \( b = 1.02 \), as suggested in Ref.[1]. Thus, the flame area and volume are

\[ A_f = \pi D \left( \frac{D}{2} + L_f \right) \]  
\[ V_f = \frac{1}{4} \pi D^2 L_f \]
respectively.

3. Heat release and soot formation
Heat release rate in flaming combustion (\( \dot{Q}_A \)) has convective and radiative component (\( \dot{Q}_C \) and \( \dot{Q}_R \)). They are directly proportional to the mass burning rate of fuel \( \dot{m} \) and the combustion efficiencies \( \chi \), i.e.

\[ \dot{Q}_A = \chi_A \dot{m} \Delta H_T \]  
\[ \dot{Q}_C = \chi_C \dot{m} \Delta H_T \]  
\[ \dot{Q}_R = \chi_R \dot{m} \Delta H_T \]  

Soot particles are produced as a result of incomplete combustion. It is assumed here that the particles are uniformly distributed within a flame, and few of them are consumed when they pass into oxidative regions of the flame. Therefore, the soot volume fraction \( f_v \) is

\[ f_v = \frac{\eta_v \dot{m} k_s}{\rho_s V_f} \]  

where \( \rho_s = 1100 \, \text{kg/m}^3 \), as suggested in Ref.[7], is used. The value of \( f_v \) is generally about \( 10^{-6} \).

In the equations of (7), (8), (9) and (10), the combustion efficiencies \( \chi_A \), \( \chi_C \) and \( \chi_R \), and the generation efficiency of soot \( \eta_v \), are functions of equivalence ratio \( \Phi \). The effect of ventilation on these efficiencies, as shown in Fig.1 and Fig.2, was examined through a series of tests by using the FMRC PCFS Apparatus and the 0.022 m^3 Enclosure at the Fire Research Institute, Mitaka, Tokyo, Japan,[8] and can be ex-
pressed as the \( \Gamma \)-correlations, i.e.

\[
\begin{align*}
\chi_A &= \chi_{A0} (1 + \Gamma_A) \\
\chi_C &= \chi_{C0} (1 + \Gamma_C) \\
\chi_R &= \chi_A - \chi_C = \chi_{R0} + \chi_{A0} \Gamma_A - \chi_{C0} \Gamma_C \\
\eta_r &= \eta_{r0} (1 + \Gamma_S)
\end{align*}
\]  

(11) \hspace{2cm} (12) \hspace{2cm} (13) \hspace{2cm} (14)

where the \( \chi_{A0}, \chi_{C0}, \chi_{R0} \) and \( \eta_{r0} \) are combustion efficiencies and generation efficiency of soot at well-ventilated conditions respectively. The

\[
\Gamma_i = \alpha_i \exp(-\beta_i \Phi^{-\delta_i})
\]

is defined as the ventilation-controlled combustion parameter, \( i = A, C, S \), the coefficients \( \alpha_i, \beta_i \) and \( \delta_i \) are constants, and are listed in the Table 1 and Table 2. Substituting \( \chi_R \) and \( \chi_C \) from Equation (2) and (13) into Equation (9) gives the relationship between \( \dot{Q}_R \) and \( \Phi \), i.e.

\[
\dot{Q}_R = \frac{E \chi_{\text{air}}} {k_a} \Delta H_T (\chi_{R0} + \chi_{A0} \Gamma_A - \chi_{C0} \Gamma_C) \Phi
\]  

(15)

4. Flame radiative properties

If emission from the molecular emitters is ignored, the flame emissivity depends only on the concentration and characteristics of soot particles and on the mean beam length of the flame, and can be expressed as

\[
\varepsilon = 1 - \exp(-KL)
\]  

(16)

where \( K \) is the effective emission coefficient, proportional to the concentration and radiative temperature of soot particles. A mean effective emission coefficient is suggested as\(^\text{[9]}\)

\[
\begin{array}{|c|c|c|c|}
\hline
\text{Table 1. Correlation coefficients} & \alpha & \beta & \xi \\
\hline
\Gamma_A & -0.97 & 2.5 & 1.2 \\
\Gamma_C & -1.00 & 1.2 & 1.8 \\
\hline
\end{array}
\]
\[ K = 3.72 \frac{C_0}{C_2} f, T_f \] \hspace{1cm} (17)

where \( C_0 \) is a constant between 2 and 6, depending on the complex index of refraction. \( C_2 \) is the Planck's second constant (1.4388 \times 10^{-2} \text{ m} \cdot \text{K}). The definition of the mean beam length for flame volumes is \[ L = 3.6 \frac{V_f}{A_f} \] \hspace{1cm} (18)

If the inlet air flow rate \( \dot{m}_{\text{air}} \) and burning area \( A_v \) (or diameter of fuel bed \( D \)) are given, substituting \( A_v, \dot{Q}_R \) and \( \varepsilon \) from Equation (5), (15), and (16) into Equation (1), the functional relationship between \( T_f \) and \( \Phi \) can be obtained.

<table>
<thead>
<tr>
<th>Table 2. Data used in the prediction</th>
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<tbody>
<tr>
<td>PMMA</td>
</tr>
<tr>
<td>( \alpha )</td>
</tr>
<tr>
<td>( \beta )</td>
</tr>
<tr>
<td>( \xi )</td>
</tr>
<tr>
<td>( x_{A0} )</td>
</tr>
<tr>
<td>( x_{C0} )</td>
</tr>
<tr>
<td>( n_{e0} )</td>
</tr>
<tr>
<td>( k_a )</td>
</tr>
<tr>
<td>( k_b )</td>
</tr>
<tr>
<td>( \Delta H_T ) (kJ / g)</td>
</tr>
</tbody>
</table>

RESULT AND DISCUSSION

According to the experiments performed at the FMRC, USA and the Fire Research Institute, Japan, the following polymers were selected in this study.

(1) Carbon–hydrogen containing polymers:
   a) aliphatic: polyethylene, \{\( (C_2H_4)_n \}\] and polypropylene, \{\( (C_3H_6)_n \}\];
   b) aromatic: polystyrene, \{\( (C_8H_8)_n \}\];

(2) Carbon–hydrogen–oxygen containing polymers (aliphatic only):
   polymethylmethacrylate, \{\( (C_5H_8O_2)_n \}\] and pine wood crib, \{\( (C_8H_{10}O_2)_n \}\];

(3) Carbon–hydrogen–oxygen–nitrogen containing polymer (aliphatic only):
   nylon, \{\( (C_{12}H_{22}O_2N_2)_n \}\].

The calculation was carried out in the following two cases. For small–scale fires, \( \dot{m}_{\text{air}} = 1.36 \text{ g/s} \), \( A_v = 70.88 \text{ cm}^2 \), in the light of experimental conditions of the
FMRC PCFS Apparatus. For large-scale fires, a real room with an opening of 1.2m × 1.5m (height) and burning area of 3.6 m² was considered, the inlet air flow rate may be given by Equation (3), i.e. \( m_{\text{air}} = 1.146 \text{ kg/s} \). The other data used in the prediction are listed in the Table 2. The results are shown in Fig.3 to Fig.11.

Fig. 3 Dependence of \( \dot{Q}_A \) and \( \dot{Q}_R \) on \( \Phi \)  
Fig. 4 Dependence of \( f_\nu \) on \( \Phi \)  
Fig. 5 Dependence of \( T_r \) on \( \Phi \)  
Fig. 6 \( T_r \) versus \( f_\nu \) for various polymers at well-ventilated conditions

1. The effect of fire ventilation

The effects of ventilation on heat release rate, flame radiant power, soot concentration within a flame and mean flame radiative temperature are shown in Fig.3, Fig.4 and Fig.5, respectively. For well-ventilated fires, the \( \dot{Q}_A \) and \( \dot{Q}_R \) increase with mass burning rate \( \dot{m} \) very abruptly at a constant \( m_{\text{air}} \), the \( f_\nu \) and \( T_r \) are almost independent of \( \Phi \). On the other hand, for under-ventilated fires, the \( \dot{Q}_A \) and \( \dot{Q}_R \) increase slowly with \( \dot{m} \), and reach their asymptotic values gradually. The approach of \( \dot{Q}_R \) to \( \dot{Q}_A \) suggests that with reduce ventilation, higher fraction of \( \chi_A \) is converted to \( \chi_R \). Meanwhile, \( f_\nu \) increases and \( T_r \) decreases steeply as \( \Phi \) increases, due to the
imcomplete combustion and heat loss from soot particles.

2. The effect of chemical structure of polymers

From Fig.1, Fig.2 and Table 1, it can be seen that the $\Gamma_A$ and $\Gamma_C$ have the same $\alpha$, $\beta$ and $\xi$ values for all polymers in this study, therefore, the fractions of $X_A/X_{A0}$ and $X_C/X_{C0}$ are expected to be independent of the chemical structures of the fuels. The $\Gamma_S$, on the other hand, has different $\alpha$, $\beta$ and $\xi$ values, and the fractions of $\eta_S/\eta_{S0}$ and $\chi_R/\chi_{R0}$ depend on the chemical structures of the polymers (see Table 2 and Equation (15)).

Fig.7 $\dot{Q}_R$ as a function of $f_v$

Fig.8 Predicted $T_f$ for both scale fires

The mean flame radiative temperatures of various polymers at well-ventilated conditions are shown in Fig.6, as a function of $f_v$. It is suggested that fuels having sootier flames have lower flame temperatures. The order of $T_f$ is: wood (C–H–O structure) > PMMA (C–H–O structure) > nylon (C–H–O–N aliphatic structure) > PE (C–H aliphatic structure) $\approx$ PP (C–H aliphatic structure) > PS (C–H aromatic
The oxygen content of wood, PMMA and nylon are 49%, 32% and 14%, and the C to H ratio of PE, PP and PS are 6, 6, and 12, respectively. In addition, the order of $f_v$ is similar to the order of carbon content of the polymers, i.e. wood (44%) < PMMA (60%) < nylon (64%) < PP & PE (86%) < PS (92%). This result implies that to a certain extent $T_f$ and $f_v$ may depend on the oxygen content, carbon content or C to H ratio of fuels.

3. The effect of soot concentration

A steep rise in $\dot{Q}_R$ with $f_v$ is shown in Fig.7 for well-ventilated fires ($\Phi < 1$). Oppositely, the increase in $\dot{Q}_R$ with $f_v$ slopes more gently for under-ventilated fires ($\Phi > 1$).

4. The effect of fire scale

It was found that in large-scale fires the heat release rate and mass burning rate per unit surface area of fuel increase with fire size because of increase in the flame radiative heat flux, and finally reach their asymptotic values. The prediction of $T_f$ for both scale fires showes in Fig.8 that the $T_f$ is almost independent of fire size.

5. Comparison with the GFR Model and experiments

The Global Flame Radiation Model of de Ris and Orloff\cite{2} was also used to independently predict $\chi_R$ and $T_f$. The values predicted from the GFR Model for well-ventilated polymer fires are shown in Fig.9, which are in excellent agreement with the prediction from the present model. With slight modification of the GFR Model\cite{8}, the $\chi_R$ and $T_f$ can be predicted for under-ventilated combustions. The results for wood crib fires are shown in Fig.10 and Fig.11, compared with the experimental data and the prediction from the present model. In addition, the $T_f$ of PMMA suggested in Ref.[1] and [9] is 1573 K and 1538 K respectively, the predicted value in this study is $T_{f_{\text{max}}} \approx 1480$ K. The comparisons indicate that the present approximate model is satisfactory for prediction of $\chi_R$ and $T_f$ of polymer fires at both well- and under-ventilated conditions.
CONCLUSION

(1) The fire ventilation is an important factor affecting fire behaviors in compartment, especially at under-ventilated conditions. An approximate model for prediction of ventilation effects on flame radiation has been established, based on the $\Gamma$-correlations, and also has been found to be reasonable in comparison with the experimental data and the prediction from Global Flame Radiation Model.

(2) For under-ventilated fires, flame radiant fraction and temperature depend on the ventilation. On the other hand, for well-ventilated fires, they are almost independent of the ventilation.

(3) Global Flame Radiation Model modified slightly is satisfactory to predict flame radiant fraction and temperature for both well- and under-ventilated polymer fires.

REFERENCES


307