

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 Γ -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

A	area of compartment opening (m^2)	α	general correlation coefficient
A_f	flame area (m^2)	β	shift correlation coefficient
A_v	burning area of fuel (m^2)	Γ	ventilation-controlled combustion parameter
C	enclosure constant ($\text{kg} / \text{sm}^{5/2}$)	ϵ	flame emissivity
C_0	constant between 2 and 6	η_s	generation efficiency of soot
C_2	Planck's second constant	ξ	slope correlation coefficient
D	diameter of fuel bed (m)	ρ_s	density of soot particles (kg / m^3)
E	entrainment coefficient	σ	Stefan-Boltzmann constant
f_v	soot volume fraction	Φ	equivalence ratio
H	height of compartment opening (m)		

ΔH_T	heat of combustion (kJ / g)	χ	combustion efficiency
K	effective emission coefficient (1 / m)	Polymers:	
k_a	mass air-to-fuel stoichiometric ratio	Nylon	nylon
k_s	stoichiometric yield for maximum fuel conversion to soot	PE	polyethylene
L	mean beam length (m)	PMMA	polymethylmethacrylate
L_f	flame height (m)	PP	polypropylene
\dot{m}	mass burning rate of fuel (kg / s)	PS	polystyrene
\dot{m}_{air}	inlet air flow rate (kg / s)	WC	wood crib
\dot{Q}	heat release rate (kW)	Subscripts:	
T_f	mean flame radiative temperature (K)	A	total heat release
T_∞	ambient temperature (298.15 K)	C	convective
V_f	flame volume (m ³)	R	radiant
		0	well-ventilated

INTRODUCTION

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 10~100 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.^[1] 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.

$$\dot{Q}_R = A_f \epsilon \sigma (T_f^4 - T_\infty^4) \quad (1)$$

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]

$$\Phi = \frac{k_a \dot{m}}{E \dot{m}_{air}} \quad (2)$$

where E is the entrainment coefficient, and is estimated to be about 0.8 in the calculation of Φ . 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]:

$$\dot{m}_{air} = CA\sqrt{H} \quad (3)$$

where the value of enclosure constant C ranges from 0.40 to 0.61 $\text{kg} / \text{sm}^{5/2}$, depending on the flow coefficient of the opening. The commonly used value is 0.52 $\text{kg} / \text{sm}^{5/2}$.

2. Flame size and shape

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

$$L_f = a\dot{Q}_A^{2/5} - bD \quad (4)$$

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

$$A_f = \pi D \left(\frac{D}{2} + L_f \right) \quad (5)$$

$$V_f = \frac{1}{4} \pi D^2 L_f \quad (6)$$

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 χ , i.e.

$$\dot{Q}_A = \chi_A \dot{m} \Delta H_T \quad (7)$$

$$\dot{Q}_C = \chi_C \dot{m} \Delta H_T \quad (8)$$

$$\dot{Q}_R = \chi_R \dot{m} \Delta H_T \quad (9)$$

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

$$f_v = \frac{\eta_s \dot{m} k_s}{\rho_s V_f} \quad (10)$$

where $\rho_s = 1100 \text{ kg} / \text{m}^3$, 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 χ_A , χ_C and χ_R , and the generation efficiency of soot η_s , are functions of equivalence ratio Φ . 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 Γ -correlations, i.e.

$$\chi_A = \chi_{A0} (1 + \Gamma_A) \tag{11}$$

$$\chi_C = \chi_{C0} (1 + \Gamma_C) \tag{12}$$

$$\chi_R = \chi_A - \chi_C = \chi_{R0} + \chi_{A0}\Gamma_A - \chi_{C0}\Gamma_C \tag{13}$$

$$\eta_s = \eta_{s0} (1 + \Gamma_S) \tag{14}$$

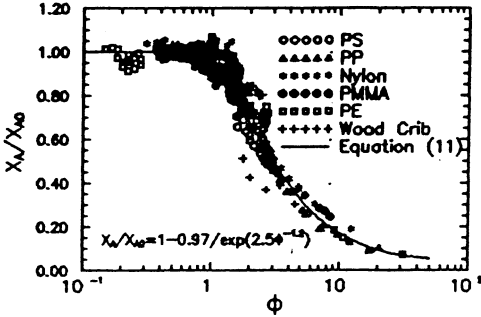


Fig.1 The effect of ventilation on χ_A

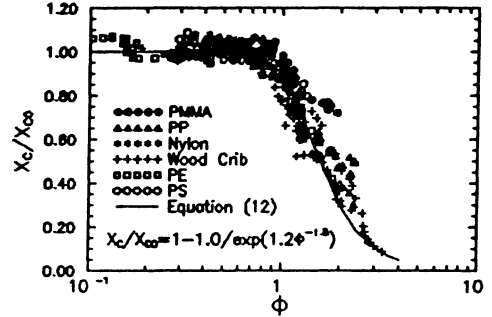


Fig.2 The effect of ventilation on χ_C

where the χ_{A0} , χ_{C0} , χ_{R0} and η_{s0} are combustion efficiencies and generation efficiency of soot at well-ventilated conditions respectively. The $\Gamma_i = \alpha_i \exp(-\beta_i \Phi^{-\xi_i})$ is defined as the ventilation-controlled combustion parameter, $i = A, C, S$, the coefficients α_i , β_i and ξ_i are constants, and are listed in the Table 1 and Table 2. Substituting \dot{m} and χ_R from Equation (2) and (13) into Equation (9) gives the relationship between \dot{Q}_R and Φ , i.e.

Table 1. Correlation coefficients

	α	β	ξ
Γ_A	-0.97	2.5	1.2
Γ_C	-1.00	1.2	1.8

$$\dot{Q}_R = \frac{E \dot{m}_{air} \Delta H_T}{k_a} (\chi_{R0} + \chi_{A0}\Gamma_A - \chi_{C0}\Gamma_C) \Phi \tag{15}$$

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

$$\varepsilon = 1 - \exp(-KL) \tag{16}$$

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^[9]

$$K = 3.72 \frac{C_0}{C_2} f_v T_f \quad (17)$$

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^[10]

$$L = 3.6 \frac{V_f}{A_f} \quad (18)$$

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

Table 2. Data used in the prediction

	PMMA	Nylon	PE	PP	WC	PS
α_s	1.6	1.7	2.2	2.2	2.5	2.8
β_s	2.5	2.5	2.5	2.5	2.5	2.5
ξ_s	0.6	0.8	1.0	1.0	1.2	1.3
χ_{A0}	0.95	0.89	0.88	0.87	0.86	0.72
χ_{C0}	0.65	0.55	0.54	0.52	0.50	0.30
η_{s0}	0.031	0.048	0.060	0.060	0.013	0.158
k_a	8.24	11.19	14.72	14.72	6.25	13.22
k_s	0.600	0.634	0.857	0.868	0.530	0.923
ΔH_T (kJ/g)	25.2	30.8	43.6	43.4	17.9	39.2

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, $\{(C_6H_{10}O_5)_n\}$;

(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. $\dot{m}_{air} = 1.146 \text{ kg/s}$. The other data used in the prediction are listed in the Table 2. The results are shown in Fig.3 to Fig.11.

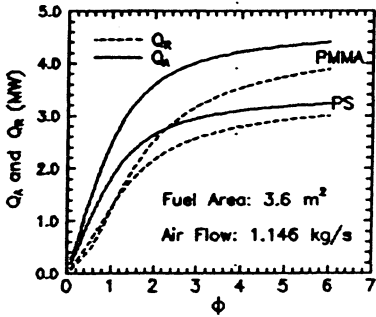


Fig. 3 Dependence of \dot{Q}_A and \dot{Q}_R on Φ

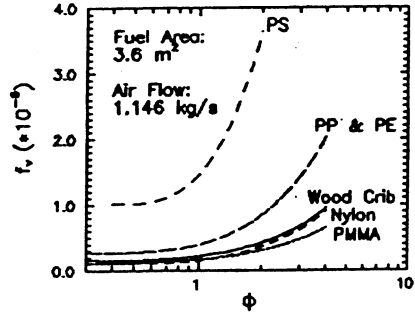


Fig. 4 Dependence of f_v on Φ

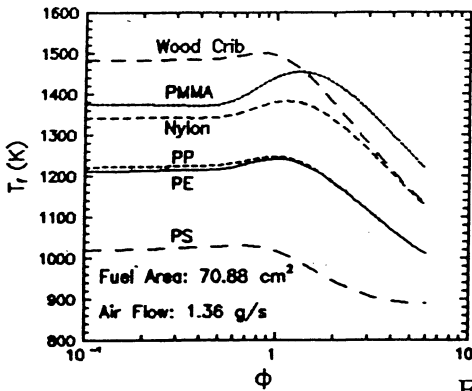


Fig. 5 Dependence of T_f on Φ

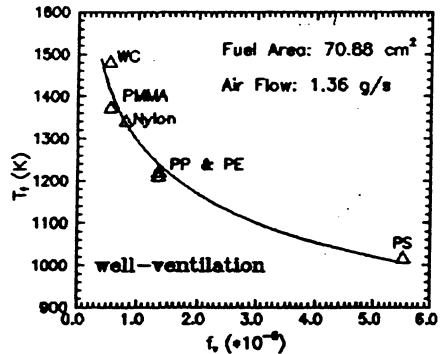


Fig. 6 T_f versus f_v for various polymers at well-ventilated conditions

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 \dot{m}_{air} , the f_v and T_f are almost independent of Φ . 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 χ_A is converted to χ_R . Meanwhile, f_v increases and T_f decreases steeply as Φ increases, due to the

incomplete 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 Γ_A and Γ_C have the same α , β and ξ values for all polymers in this study, therefore, the fractions of χ_A / χ_{A0} and χ_C / χ_{C0} are expected to be independent of the chemical structures of the fuels. The Γ_S , on the other hand, has different α , β and ξ values, and the fractions of η_s / η_{s0} and χ_R / χ_{R0} depend on the chemical structures of the polymers (seeing Table 2 and Equation (15)).

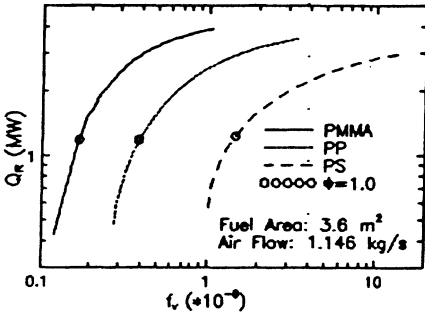


Fig.7 \dot{Q}_R as a function of f_v

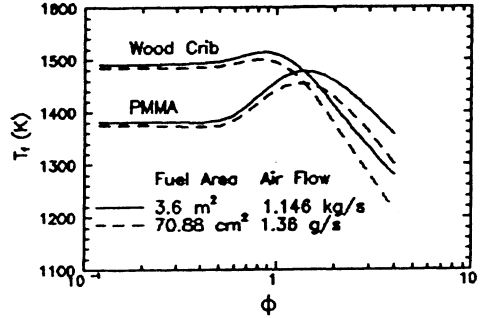


Fig.8 Predicted T_f for both scale fires

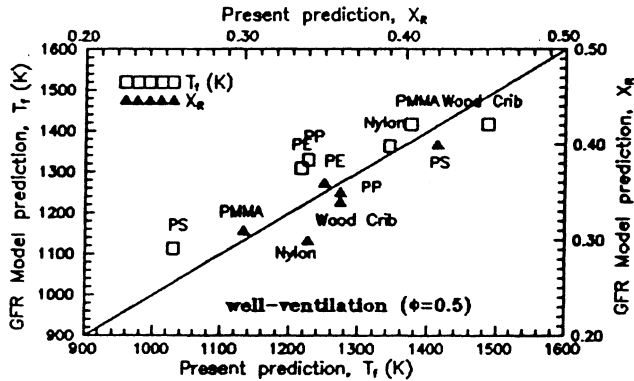


Fig.9 Predicted T_f and χ_R for well-ventilated combustion

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

structure). 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.^{[3],[11]} The prediction of T_f for both scale fires shows 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^[2] was also used to independently predict χ_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^[8], the χ_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 $T_{fmax} \approx 1480$ K. The comparisons indicate that the present approximate model is satisfactory for prediction of χ_R and T_f of polymer fires at both well- and under-ventilated conditions.

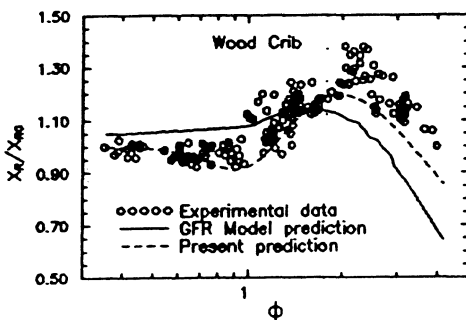


Fig.10 Comparison of predicted χ_R with the experimental data

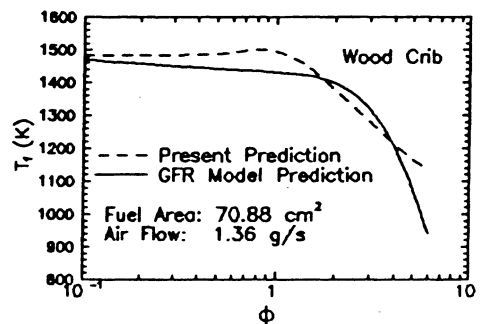


Fig.11 Comparison of predicted T_f

CONCLUSION

- (1) The fire ventilation is an important factor affecting fire behaviors in a compartment, especially at under-ventilated conditions. An approximate model for prediction of ventilation effects on flame radiation has been established, based on the Γ -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.

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