

Estimation of Heat Release in Fire Compartment

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ABSTRACT

This paper presents the model to estimate heat release in fire compartment about four fuels, Douglas fir considering char formation and moisture content, methanol, methane and propane, with equivalence ratio ϕ on the basis of previous work and discusses about the difference of the combustion efficiency of them.

As the result, calculated heat release of Douglas fir, methane and propane shows relatively good relation to previous work. By considering the differences of combustion efficiency of fuels, we will be able to conduct the experiments with many fuels to examine heat balance of compartment fire. And the results of combustion efficiency of four fuels show that in $\phi \leq 1$, combustion efficiency of Douglas fir, methanol, methane and propane are almost same, but in $\phi > 1$ as ϕ increases, as combustion efficiency of them differ largely. The reason is considered that heat of reaction is consumed to latent heat of non-reacted fuel in accordance with the amount of non-reacted fuel.

NOMENCLATURE

ΔH_{fx} : heat of formation of completely burned gas of dry fuel (kJ/kg)

ΔH_f : heat of formation of chemical species i (kJ/kg)

ΔH_{fs} : heat of formation of dry fuel (kJ/kg)

$\Delta H_x'$: enthalpy of pyrolysis gas (kJ/kg weight loss)

ΔH_{fx} : heat of formation of burned gas in arbitrary condition (kJ/kg)

Δh_m : heat of formation divided in proportion to the amount of oxygen in fuel and air (kJ/kg)

Q_f : heat release in arbitrary condition (kJ/kg)

Q_c : heat of combustion (kJ/kg)

$Q_{c,wz}$: heat of combustion except for char and moisture content (kJ/kg)

$Q_{c,w}$: heat of combustion except for moisture content (kJ/kg)

q_{O_2} : heat release per gram of oxygen in air consumed (kJ/g O₂)

x_C', x_H', x_O', x_N' : mass fractions of C, H, O and N (kg/kg dry fuel)

x_z' : char ratio (kg/kg dry fuel)
 x_w' : moisture content (kg/kg wet fuel)
 a, b, c, d : mole numbers of C, H, O and N of dry fuel (mole)
 CE : combustion efficiency (-)
 k : combustion efficiency defined by Hamada (-)
 L_{dry} : latent heat of dry fuel (kJ/kg weight loss)
 \dot{m}_f, \dot{m}_a : mass rate of fuel and air (kg/s)
 n : excess air ratio (-)
 r, s, p_1, p_2, q_1 : the coefficients (-)
 ϕ : equivalence ratio (-)
 ϕ_s : stoichiometric reacting fuel to air ratio (-)

INTRODUCTION

A lot of studies concerning about compartment fire have been done. Sekine[1] modeled the temperature in fully developed fire compartment. Then many fire models have been developed. In these models, heat release rate has been evaluated as the product of weight loss rate and heat of combustion of the combustibles[2,3] or heat release considering empirical combustion efficiency[1,4-7]. But little studies have been done about heat release of fuels, such as wood, considering char formation and moisture content to influence them.

To study the properties of compartment fire, many experiments using small-scale model had been done. Besides the cellulosic materials, which are the main combustibles of actual fire, liquid and gaseous fuel had been used as the fuel in experiments because of the ease to handle and the definite properties. But it has not been well discussed about the differences among them.

This paper presents the results of the estimated heat release of Douglas fir considering char formation and moisture content, methanol, methane and propane, with equivalence ratio on the basis of previous work and discusses about the difference of the combustion efficiency of them.

PREVIOUS WORK

Recently many plastic materials have come into use in buildings, but it has been reported that the main combustibles were woody materials[8,9]. The summary of previous work concerning about pyrolysis, gas composition of burned gas and heat release of these materials is shown as below.

Most part of woody materials consists of cellulose, hemicellulose and lignin, so combustion of cellulose has been studied mainly as that of wood. Although a lot of studies concerning about the combustion of cellulose, related to the problem of energy, incineration of garbage and fire safety, have been done[10,11], it is not easy to evaluate its combustibility quantitatively. The pyrolysis of cellulose is complicated physically and chemically, and the composition of char, soot and the volatile is influenced by atmospheric condition. Char changes its composition with the increase of temperature and duration of heating, so it is difficult to specify its composition and the nature. The experimental results show that char is formed by 0 ~ 30% weight of initial cellulose[12-15].

On the point of gas toxicity, Beyler[16,17] studied CO, CO₂, H₂ and O₂ yield with equivalence ratio by small scale experiments to burn 13 kinds of fuels under hood steadily. Then Gottuk et al[18] conducted large scale experiments and showed the same property. Zukoski et al[19] examined those in transient state. From Beyler's results, Yamada-Tanaka[20] assumed that the normalized yield of

chemical species of propane could be regarded as the same for all fuels, and made a model for predicting the yields of chemical species. However, it was shown that there is influence of temperature of hot gas layer on the composition of the gas [16,18,19], it has not been well discussed and modeled.

Tewarson [21] tried to quantify the generation efficiency of heat and chemical species with a lot of experimental results in fully developed compartment fire, but it was not enough to make a model.

Hamada [4] derived that heat release of wood in fire compartment was shown as $10298k+4596$ (kJ/kg) by using Dulong's formula assuming the generation ratio of CO₂ and CO to be k and $1-k$ respectively. Kawagoe [22] conducted fire experiments using 10 kinds of full size building and concluded that the combustion efficiency k was about $0.5 \sim 0.8$ and excess air ratio n was $0.8 \sim 1.2$ from measured gas composition at the opening during the period of fully developed fires. On the basis of these results, Sekine [1] and Kawagoe·Sekine [5] estimated temperature in fully developed fire compartment by solving energy balance with $k=0.6$ and $n=1.0$. Then Harmathy [6] evaluated heat release in fire compartment with two factors. One is reaction efficiency due to the formation of CO and soot, and the other is mixing factor due to incomplete mixing between air and pyrolysis gases. These factors have been used in many studies, but they had not been well discussed.

Nakaya [7] made a model using computer program to predict the yield of chemical species, temperature and combustion inefficiency of burned gas of wood in fire compartment with equivalence ratio as a variable. Then he compared the calculated CO, CO₂ and O₂ yields with Tewarson's data and concluded that a fairly good agreement had been obtained. His study is based on the experimental results of Ohlemiller et al [23], but they are applicable to limited situation. Because the experiments were conducted to analyze gas composition without combustion and there was the influence of moisture content for the balance of chemical species. Moreover, in case of pyrolysis of cellulosic materials, it has been reported that the pyrolysis gases prevent the oxygen from diffusing to fuel surface even though temperature is lower than that to ignite. So it can be considered that there is no large difference between wood pyrolysis in the air and that in the inert gases [10].

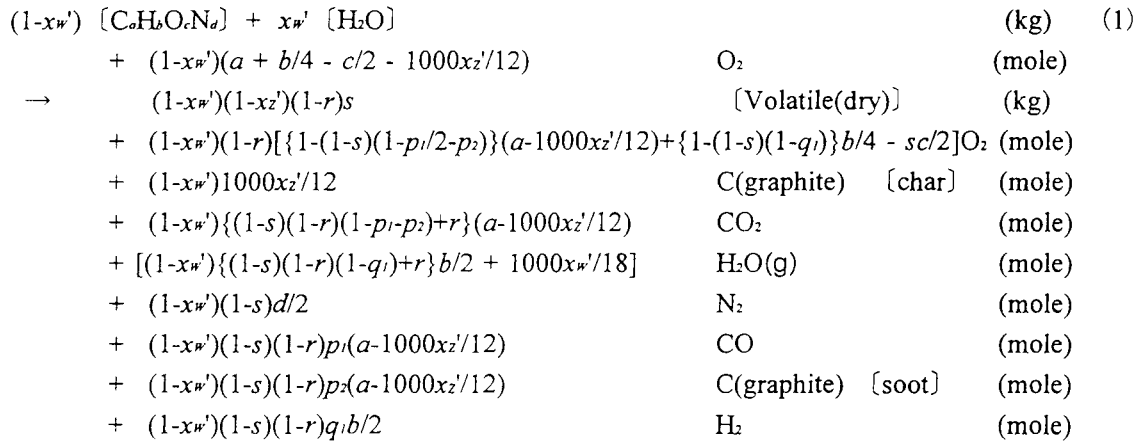
Hugget [24] showed that heat release per gram of oxygen consumed were approximately the same for most fuels commonly encountered in fire. And he mentioned that even though the 10% of the carbon became CO, heat loss was very small.

CALCULATION OF HEAT RELEASE

Based on previous studies, to calculate heat release of cellulose or wood, we assumed as below.

Fuel is composed of carbon, hydrogen, oxygen and nitrogen. Char is formed by carbon graphite in the process to pyrolyze, and soot is generated by carbon graphite in the process of combustion. Char ratio x_2' is 20% of the weight of initial fuel in dry state. Latent heat L_{23}' of dry fuel is constant regardless of char formation. The combustibilities of wood are equivalent to that of cellulose. There is no generation of O₂ and NO_x from fuel pyrolysis and no coagulation of tar. Besides the process of fuel pyrolysis, the yield of chemical species of burned gas can be expressed as model of Yamada·Tanaka [20]. Moisture content $x_{w'}$ is 13% in unit of wet wood as the mean of air dry wood and general covering materials [25]. There is no effect of moisture on combustion. The air is composed of 21% oxygen and 79% nitrogen. There is no consideration about the enthalpy accumulating in burned gas with temperature rise and the work with volumetric change.

Letting a , b , c and d be mole numbers of C, H, O and N in dry fuel respectively. The combustion formula of unit of weight fuel and coefficients are shown as next.



Here x_c' , x_H' , x_o' and x_N' are the mass fractions of C, H, O and N of dry fuel respectively, so mole numbers are shown as Eq.(2).

$$a = 1000x_c'/12, \quad b = 1000x_H', \quad c = 1000x_o'/16, \quad d = 1000x_N'/14 \quad \text{(mole)} \quad (2)$$

Then heat release in arbitrary state shown by equivalence ratio can be calculated as below.

First of all, we calculate heat of formation of completely burned gas $\Delta H_{f_{cg}}$ of dry fuel to sum up heat of formation of chemical species i , ΔH_{f_i} from x_c' , x_H' , x_o' and x_N' by Eq.(3). Using heat of combustion Q_c and latent heat, heat of formation of dry fuel $\Delta H_{f_{cs}}$, heat of formation of wet fuel $\Delta H_{f_{fw}}$ and enthalpy of pyrolysis gas ΔH_{f_g} can be derived from Eq.(4) ~ (6) respectively. Using formula(1), heat of formation of burned gas in arbitrary condition, $\Delta H_{f_{cg}}$, can be calculated from Eq.(3). Then considering heat of formation of moisture content, heat release in arbitrary condition Q_f can be derived from Eq.(7).

$$\Delta H_{f_{cg}} = \sum_i (v_i'' - v_i') \Delta H_{f_i} \quad \text{(kJ/kg)} \quad (3)$$

$$\Delta H_{f_{cs}} = \Delta H_{f_{cg}} + Q_c \quad \text{(kJ/kg)} \quad (4)$$

$$\Delta H_{f_{fw}} = (1-x_w') \Delta H_{f_{cs}} + (1000x_w'/18) \times (-285.988) \quad \text{(kJ/kg)} \quad (5)$$

$$\Delta H_{f_g} = \Delta H_{f_{cs}} + L_{vs}' \quad \text{(kJ/kg)} \quad (6)$$

$$Q_f = -\Delta H_{f_{cg}} + \Delta H_{f_{fw}} \quad \text{(kJ/kg)} \quad (7)$$

From stoichiometric fuel to air ratio ϕ_s , mass rate of fuel \dot{m}_f and mass rate of air \dot{m}_a , equivalence ratio ϕ is defined as Eq(8).

$$\phi = \frac{\dot{m}_f}{\phi_s \dot{m}_a} \quad (8)$$

Here ϕ_s is defined by the fuel to react in gas phase and also in surface combustion, if there. Then $\Delta H_{f_{cg}}$ can be given as Eq.(9) and (10).

(1) In case of $\phi \leq 1$ (air rich condition),

$$\begin{aligned}
\Delta H_{fg} = & (1-x_w')\{(1-s)(1-r)(1-p_1-p_2)+r\}(a-1000x_z'/12) & \times (-393.693) & : \text{CO}_2 \\
& + (1-x_w')\{(1-s)(1-r)(1-q_1)+r\}b/2 & \times (-241.951) & : \text{H}_2\text{O(g)} \\
& + (1-x_w')(1-s)(1-r)p_1(a-1000x_z'/12) & \times (-110.594) & : \text{CO} \\
& + 1000x_w'/18 & \times (-241.951) & : \text{H}_2\text{O(g)} \\
& + (1-x_w')(1-x_z')(1-r)s & \times \Delta H_g' & : [\text{Volatile(dry)}] .
\end{aligned} \tag{9}$$

(2) In case of $\phi > 1$ (fuel rich condition),

$$\begin{aligned}
\Delta H_{fg} = & (1-x_w')\{(1-s)(1-r)(1-p_1-p_2)+r\}(a-1000x_z'/12)/\phi & \times (-393.693) & : \text{CO}_2 \\
& + (1-x_w')\{(1-s)(1-r)(1-q_1)+r\}b/(2\phi) & \times (-241.951) & : \text{H}_2\text{O(g)} \\
& + (1-x_w')(1-s)(1-r)p_1(a-1000x_z'/12)/\phi & \times (-110.594) & : \text{CO} \\
& + 1000x_w'/18 & \times (-241.951) & : \text{H}_2\text{O(g)} \\
& + (1-x_w')(1-x_z')\{(1-r)s/\phi+(1-1/\phi)\} & \times \Delta H_g' & : [\text{Volatile(dry)}] .
\end{aligned} \tag{10}$$

Then heat release per gram of oxygen in air consumed q_{O_2} can be calculated by Eq.(11). Fuels, like wood or cellulose, have oxygen in their molecule. When these fuels burn, heat of reaction of oxygen in air will be different how the oxygen in fuel combines carbon, hydrogen and compounds in burned gases, because there is difference between heat of formation of CO_2 and that of H_2O . Actually there is recombination in the process of reaction, so it is difficult to predict how much and what kinds of species the oxygen in air reacts. We assume that heat of formation of burned gas is divided in proportion to the amount of oxygen in fuel and air to react. Then the value of heat of formation which generated by oxygen in fuel Δh_m is expressed by Eq.(12). Here Δh_g is the sum from first to third term of Eq.(9) and(10).

$$q_{O_2} = \frac{Q_f}{(1-x_w')\{(a+b/4-c/2-1000x_z'/12)-(1-r)[\{1-(1-s)(1-p_1/2-p_2)\}(a-1000x_z'/12) + \{1-(1-s)(1-q_1)b/4\}-sc/2\}]\} \times 32 \times \begin{cases} 1 & (\phi < 1) \\ \phi & (\phi \geq 1) \end{cases} \text{ (kJ/gO}_2\text{)} \tag{11}$$

$$\Delta h_m = \Delta h_g \frac{\{1-(1-r)s\}c/2}{\{r+(1-s)(1-r)(1-p_1/2-p_2)\}(a-1000x_z'/12)+\{r+(1-q_1)(1-s)(1-r)\}b/4} \text{ (kJ/kg)} \tag{12}$$

Following the expression of Yamada·Tanaka[20], the coefficients r , s , p_1 , p_2 and q_1 are rearranged as Eq.(13) and (14) on the basis of formula (1). Here the coefficients of $\phi = 2$ are substituted for that of $\phi > 2$, as Yamada·Tanaka[20] did.

(1) In case of $\phi \leq 1$ (air rich condition),

$$r = 1-0.25^{(1/\phi)^2}, \quad s = 0.4, \quad p_1 = 0.6, \quad p_2 = 0.1, \quad q_1 = 0.25. \tag{13}$$

(2) In case of $\phi > 1$ (fuel rich condition),

$$r = 0.75, \quad s = 1-0.6^{(1/\phi)^2}, \quad p_1 = 0.6\phi^2, \quad p_2 = 0.1, \quad q_1 = 0.25\phi^2. \tag{14}$$

RESULTS AND DISCUSSION

We used the data of mass ratio, moisture content x_w' , char ratio x_z' , heat of combustion Q_f and latent heat L_{vs}' of Douglas fir, methanol, methane and propane from previous work as shown in Table 1. There are no large differences of mass ratio, heat of combustion and latent heat among general woods, so we chose Douglas fir as the representative of woods.

Table 1 Data of fuel for calculation

	Douglas Fir	Methanol	Methane	Propane
x_c' (kg/kg Fuel)	0.523 ²⁴⁾	0.375	0.750	0.8182
x_n' (kg/kg Fuel)	0.063 ²⁴⁾	0.125	0.250	0.1818
x_o' (kg/kg Fuel)	0.405 ²⁴⁾	0.500	0	0
x_n' (kg/kg Fuel)*	0.009 ²⁴⁾	0	0	0
x_w' (kg/kg wet fuel)	0.13	—	—	—
x_z' (kg/kg dry fuel)	0.2	—	—	—
Q_f (kJ/kg dry fuel)	19,600 ²⁴⁾	19,940 ²⁴⁾	50,030 ²⁴⁾	46,360 ²⁴⁾
L_{vs}' (kJ/kg weight loss)	1,820 ²⁵⁾	1,101 ²⁴⁾	—	—

* N is including other elements except for C, H and O.

Heat Release

Calculated results are shown in Fig.1 ~ 4. In Fig.1 ~ 4, heat loss by incomplete combustion starts from $\phi=0.4$, because of the definition of coefficient. In general, it is needed for complete combustion to mix air with fuel, like coal and wood, uniformly in the proportion of $n=1.4 \sim 2.0$ [26]. There is the relation of $n=1/\phi$, so complete combustion occurs at $\phi=0.5 \sim 0.7$ and below. Calculated result shows that heat loss by incomplete combustion for $\phi=0.6$ is less than 2%, there is no discrepancy between calculated result using equivalence ratio and experimental results using excess air ratio.

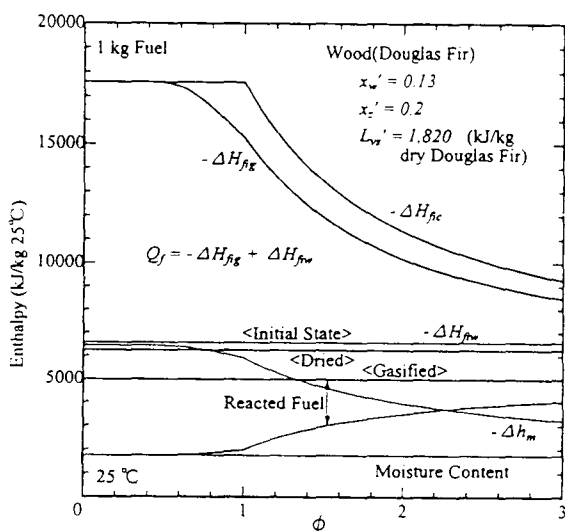


Fig.1 Enthalpy of combustion of Douglas Fir

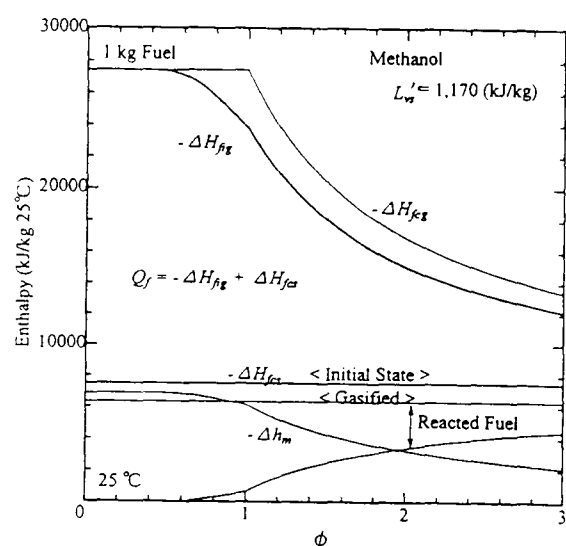


Fig.2 Enthalpy of combustion of methanol

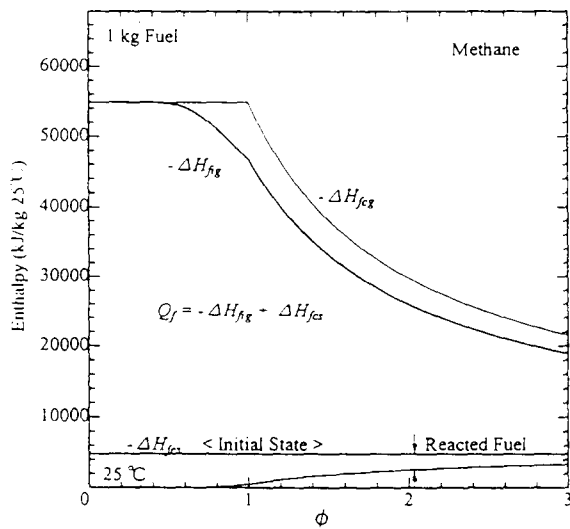


Fig.3 Enthalpy of combustion of Methane

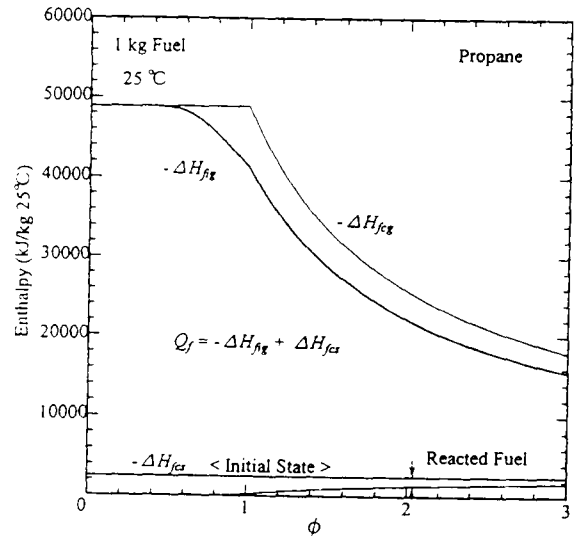


Fig.4 Enthalpy of combustion of propane

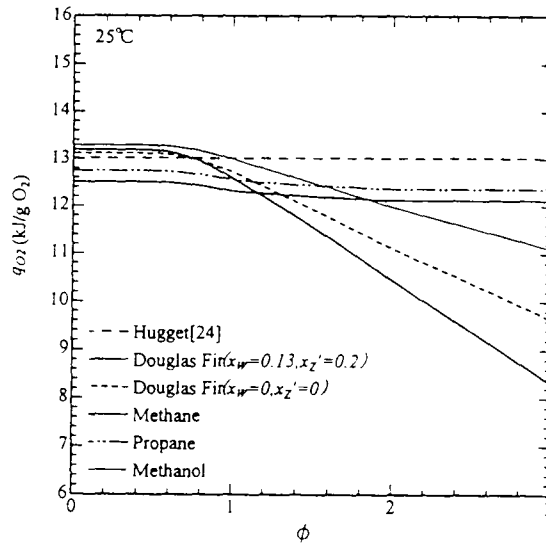


Fig.5 Heat release per gram of oxygen in air consumed

Sekine[1] used $n=1.0$, $k=0.6$ and $10,779$ (kJ/kg) for unit of weight loss of wood to calculate the temperature in fully developed fire compartment, although he did not take account for moisture content in wood. Calculated heat release of Douglas fir for $\phi=1.0$ shows $10,521$ (kJ/kg) for unit of weight loss. In spite of different condition to calculate, the values themselves are almost same.

As for Douglas fir, $-\Delta h_m$ is shown in Fig.1. It is found that the total amount of heat of formation of burned gas for lower ϕ , which oxygen contained in fuel has, is almost equal to heat of formation of initial Douglas fir. Only from the ratio of reacted oxygen, heat of reaction of oxygen in air becomes heat release as the concept of oxygen consumption method. The relation between heat release per unit of

oxygen in air consumed q_{O_2} and ϕ is shown in Fig.5. For $\phi \geq 0.6$, enthalpy generated by reaction of oxygen in air is used to pyrolysis of fuel, so q_{O_2} decreases, as ϕ increases.

As for methanol, there is same tendency as Douglas fir. And as for methane and propane, calculated enthalpy is very simple and heat release per unit of oxygen in air consumed is invariable with ϕ .

Combustion Efficiency

Various definitions for combustion efficiency had been given[7,21,22,29]. As for wood, combustion efficiency will vary in whether to choose which of heat of combustion of pyrolysis gas, initial fuel or dry fuel for denominator, because of char formation and moisture content. If we focus on heat release in fire compartment, combustibility of pyrolysis gas instead of initial fuel will be important to consider heat balance except for surface combustion of residue or char. In many previous work, it is calculated by using heat of combustion of dry fuel for denominator. Practically there is moisture content to dilute pyrolysis gas and to consume heat release in latent heat. So we defined two combustion efficiency CE as Eq.(15) and (16). Here $Q_{s,wz}$ is heat of combustion except for char and moisture content and $Q_{s,w}$ is that except for moisture content.

$$CE1 = Q_f / Q_{s,wz} \quad (15)$$

$$CE2 = Q_f / Q_{s,w} \quad (16)$$

In case of no formation of char and no moisture content, $CE1$ is equal to $CE2$.

Calculated results of combustion efficiency of Douglas fir with and without moisture content, methanol, methane and propane are shown in Fig.6. It shows that in $\phi \leq 1$, CE of methanol, methane and propane, and $CE1$ of Douglas fir are almost same, but in $\phi > 1$, as ϕ increases, as CE of them differs largely. The reason is considered that heat of reaction is consumed to latent heat of non-reacted fuel in accordance with the amount of non-reacted fuel.

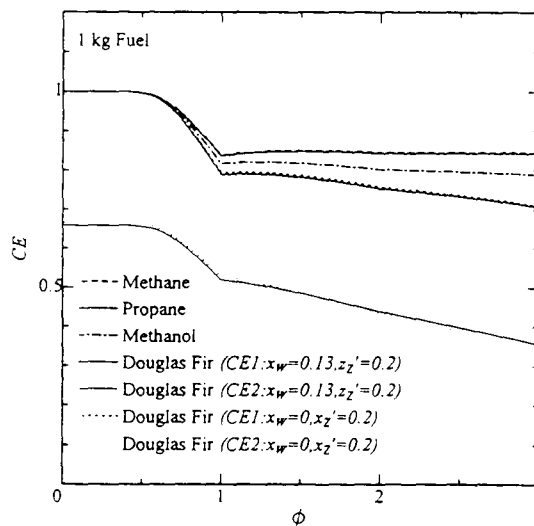


Fig.6 Comparison of Calculated results of CE

For Douglas fir with no moisture content and with formation of char, Fig.6 shows that even though pyrolysis gas burns completely or $\phi \rightarrow 0$, 68% of heat of combustion of Douglas fir with no moisture content and no formation of char is generated. This value is as almost same as experimental result of 70%, which had been conducted to burn sugar pine under hood and had been measured by oxygen consumption method by McCaffrey·Harkleroad[30], however there is no detailed description of moisture content. And they mentioned that their result had agreed with other experimental result[31].

Tewarson[21] conducted experiments to burn wood cribs and examined to compare them with other experimental results about generation efficiency of heat and chemical compounds in fully developed compartment fires. He used chemical formula of wood to be $\text{CH}_{1.5}\text{O}_{0.58}$ from measured elemental composition to define combustion efficiency as Eq.(16) with no moisture content. In this paper, we used chemical formula of Douglas fir as $\text{CH}_{1.45}\text{O}_{0.58}\text{N}_{0.01}$, this is as almost same as that of Tewarson. And it is not general to assume no formation of char in fully developed compartment fire, so we calculated combustion efficiency, assuming 20% of char formation. There is the difference of heat release by non-reacted hydrogen between them, but the difference is only about 1%. Then we compared them with Tewarson's results as shown in Fig.7. Here open marks show the experimental results which Tewarson did and solid marks show the results which Tewarson rearranged. And we compared calculated results, as shown in Fig.8, assuming char formation $x_z'=0.2$ and moisture content $x_w'=0.13$, because there were no descriptions of moisture content in his paper and the paper which he had cited. These figures show that calculated results are somewhat lower than Tewarson's results, however we may say that there are no large differences among them because of heat loss by non-reacted hydrogen and some problems, such as sampling probes in the flame, gas temperature and residence time of oxygenated compounds in hot layer, and changes in the wood decomposition mechanisms and so on, as Tewarson [21] pointed out.

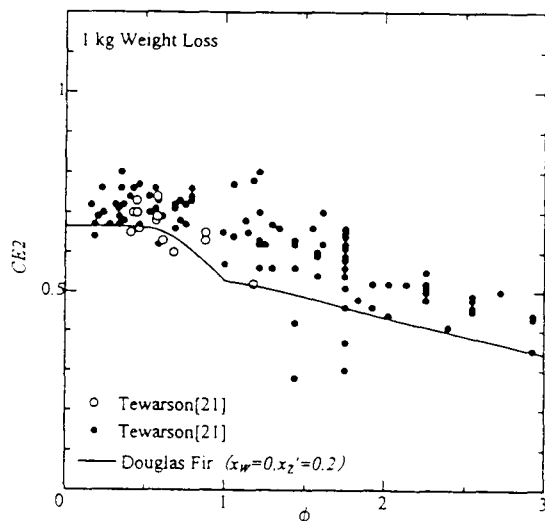


Fig.7 Relationship between previous work and calculated result 1 (Douglas Fir)

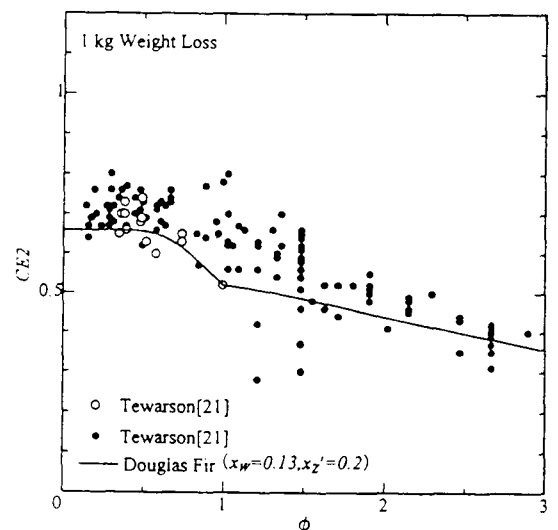


Fig.8 Relationship between previous work and calculated result 2 (Douglas Fir)

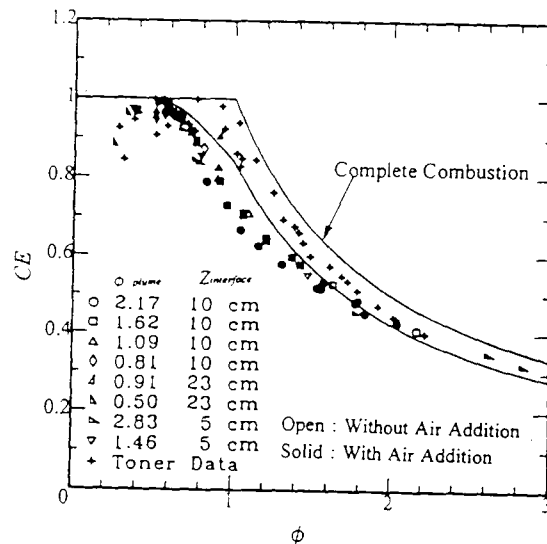


Fig.9 Relationship between previous work and calculated result 3 (methane)

Zukoski et al[19] conducted experiments to burn city gas under hood and examined the composition of chemical species of burned gas in transient state to add air to hood to change ϕ between plume and hot gas layer. Then they calculated heat release Q_f based on measured nine chemical species, O_2 , CO , CH_4 , H_2 , CO_2 , N_2 , C_2H_6 , C_2H_4 and C_2H_2 , and combustion efficiency divided by heat of combustion Q_c . The main composition of chemical species of city gas is methane (for example, 92.4 mole% [32]), so we compared their results with calculated result of methane as shown in Fig.9. However there is a little difference around $\phi = 1$, Fig.9 shows good agreement among them.

Moreover Beyler[16] mentioned that in the region of large ϕ , heat release which calculated from generation of O_2 , CO and CO_2 to burn propane was 85% of heat release calculated from consumed oxygen. In this paper we used the coefficients of Yamada Tanaka[20] based on Beyler's results[16], so there is no discrepancy between them.

CONCLUSION

We estimated heat release of four fuels, Douglas fir considering char formation and moisture content, methanol, methane and propane, with equivalence ratio on the basis of previous work and discusses about the difference of the combustion efficiency of them. Calculated results of Douglas fir, methane and propane show relatively good relation to previous work. By considering the differences of combustion efficiency of fuels, we will be able to conduct the experiments with many fuels to examine heat balance of compartment fire. On the assumption of this paper, heat release of methane and propane per gram of oxygen in air consumed are constant, but that of Douglas fir and methanol decreases, as ϕ increases. The combustion efficiency shows relatively good relation to the previous work.

We have no definite information on the chemical reaction, including the influence of temperature, residence time of hot gas layer of fire compartment on the composition of the gas and so on. It is needed further to discuss and examine on that point.

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