A NOTE ON MODELING COMBUSTION OF COMMON FUELS WITH MIXTURE FRACTION

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ABSTRACT

It is necessary to model combustion in simulating building fires more realistically while carrying out hazard assessment. The Computational Fluid Dynamics (CFD) package - Fire Dynamics Simulator (FDS) is now commonly used. The mixture fraction method is adopted in simulating combustion processes of burning materials. In this article, the mixture fraction method is reviewed. State relation of common fuels including methane, methanol, ethanol, propanol, gasoline, diesel and polymethyl methacrylate (PMMA) are calculated and reported. Results are useful in applying CFD-FDS for room fire simulations in performance-based fire safety design.

1. INTRODUCTION

Many new construction projects might have difficulties in complying with the prescriptive codes on fire safety. Performance-based design [e.g. 1] is accepted in many countries including Hong Kong [2]. Consequently, fire engineering tools such as Computational Fluid Dynamics (CFD) is widely used for hazard assessment [3]. The Fire Dynamics Simulator (FDS) [4] developed at the Building and Fire Research Laboratory, National Institute of Standards and Technology in the USA is now a popular design tool accessible to the general public. Combustion of fuels can be modelled practically by the mixture fraction method [5-8] in FDS.

In this paper, combustion modelling by the mixture fraction method will be reviewed. State function will be calculated with selected common combustibles. These included methane, methanol, ethanol, propanol, gasoline, diesel and polymethyl methacrylate (PMMA). Results are useful in applying FDS to determine fire safety provisions for big construction projects with new architectural features having difficulties to comply with prescriptive fire safety codes.

2. MIXTURE FRACTION

Given a volume containing a mixture of gas species, a mixture fraction can be defined, that is the ratio of the mass of a subset of the species to the total mass present in the volume. The mixture fraction is a conserved quantity in combustion defined traditionally as the mass fraction of the gas mixture that originates in the fuel stream. Taking the combustion of C_xH_y as an example, the mixture fraction, Z, can be defined [5,9] in terms of the mass fraction of fuel and the carbon-carrying products of combustion:

$$Z = Y_F + Y_{CO_2}\frac{W_F}{xW_{CO_2}} + Y_{CO}\frac{W_F}{xW_{CO}} + Y_{soot}\frac{W_F}{xW_{soot}} \quad (1)$$

In the above equation, W_i is the molecular weight of chemical species i, Y_i is the mass fraction of that species, x is the number of carbon atoms in the parent fuel molecule: C_xH_y, W_F is the molecular weight of the parent fuel, W_{CO_2} is 44 g/mol, W_{CO} is 28 g/mol, and W_{soot} is 12 g/mol. Alternative definitions of mixture fraction yield similar results.

The mass fraction, Y_i, of each species i is determined from the measured mole fraction, X_i, and the average molecular weight of all gas species, W_{tot}, by the following expression:

$$Y_i = X_i W_i / W_{tot} \quad (2)$$

W_{tot} is a function of the local composition, W_i, i = 1,…,N.

$$W_{tot} = \sum_i X_i W_i \quad (3)$$

The state relations [4-6] can be derived by considering the idealized reaction of a hydrocarbon fuel with air [4]:

$$C_xH_y + \eta\ (x + y/4)(O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)C_xH_y + \min(1, \eta)xCO_2 + \min(1, \eta)(y/2)H_2O + \max(0, \eta-1)(x + y/4)\ O_2 + \eta\ (x + y/4)\ 3.76N_2 \quad (4)$$

In the above equation, the function max (α, β) returns the larger of the two parameters, α or β, and the function min(α, β) returns the smaller of the two parameters, α or β. Here, η is a parameter ranging from zero (all fuel and zero oxygen) to infinity (all oxygen and zero fuel) and becomes unity for stoichiometric conditions. η is the reciprocal of the local fuel equivalence ratio, ϕ, defined in terms of the fuel-air ratio *F/A*:

$$\phi = \frac{(F/A)}{(F/A)_{st}} = \frac{W_F/\eta(x + y/4)(W_{O_2} + 3.76W_{N_2})}{W_F/(x + y/4)(W_{O_2} + 3.76W_{N_2})} = \frac{1}{\eta} \quad (5)$$

The subscript *st* in the above equation refers to the stoichiometric conditions.

The idealized mass fractions of products can be determined from the right side of Eq. (4). At the flame sheet where both the fuel and oxygen concentrations are zero, i.e. $Y_F = Y_{CO} = Y_{soot} = 0$, Z in Eq. (1) is then:

$$Z_{fs} = Y_{CO_2}\frac{W_F}{xW_{CO_2}} \quad (6)$$

3. METHANE

The mixture fraction for a methane-air flame is presented by writing the chemical reaction equation Eq. (4) as:

$$CH_4 + 2\eta\ (O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)\ CH_4 + \min(1, \eta)\ CO_2 + 2\ \min(1,\eta)\ H_2O + 2\ \max(0,\eta-1)\ O_2 + 7.52\ \eta\ N_2 \quad (7)$$

The traditional state relationship model [5,10] holds that the mass fraction, Y_i, of products can be determined from Eq. (7) as follows:

$$Y_{CH_4} = \max(0,1-\eta)W_{CH_4}/W_{tot} \quad (8a)$$

$$Y_{CO_2} = \min(1,\eta)W_{CO_2}/W_{tot} \quad (8b)$$

$$Y_{H_2O} = 2\min(1,\eta)W_{H_2O}/W_{tot} \quad (8c)$$

$$Y_{O_2} = 2\max(0,\eta-1)W_{O_2}/W_{tot} \quad (8d)$$

$$Y_{N_2} = 7.52\eta W_{N_2}/W_{tot} \quad (8e)$$

Y_{CO} and Y_{soot} in Eq. (1) were taken as zero.

The total molecular weight (W_{tot}) is a function of the local composition and was calculated from the reactant concentrations:

$$W_{tot} = W_{CH_4} + 2\eta(W_{O_2} + 3.76W_{N_2}) \quad (9)$$

Since Y_{CO} and Y_{soot} are assumed to be equal to zero and $Y_F = Y_{CH_4}$, Z in Eq. (1) can be rewritten as:

$$Z = Y_{CH_4} + Y_{CO_2}\frac{W_{CH_4}}{W_{CO_2}} \quad (10)$$

Putting Eqs. (8) and (9) into Eq. (10), Z becomes:

$$Z = \frac{W_{CH_4}}{W_{tot}} = \frac{W_{CH_4}}{W_{CH_4} + 2\eta(W_{O_2} + 3.76W_{N_2})} \quad (11)$$

And η is:

$$\eta = \frac{1-Z}{Z}\frac{W_{CH_4}}{2(W_{O_2} + 3.76W_{N_2})} = \frac{1-Z}{Z}(F/A)_{st} \quad (12)$$

Relationships between Y_i and Z for methane are plotted in Fig. 1.

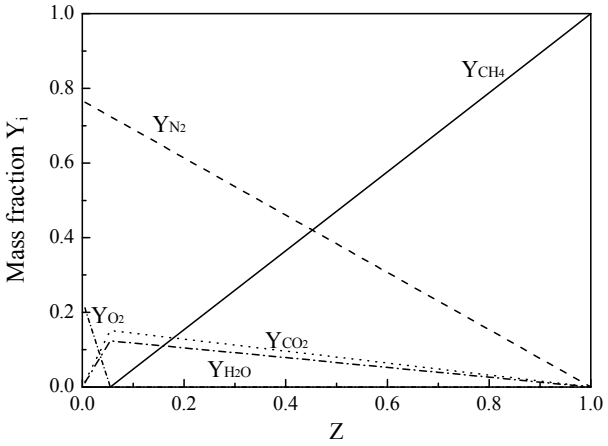

Fig. 1: State relations for methane

4. METHANOL

The global reaction of a generic oxygenated hydrocarbon fuel ($C_xH_yO_z$) with subscripts *x*, *y* and *z* being the number of carbon, hydrogen and oxygen atoms in the fuel molecule respectively with air is:

$C_xH_yO_z + \eta\ (x + y/4 - z/2)\ (O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)C_xH_yO_z + \min(1,\eta)xCO_2 + \min(1,\eta)(y/2)H_2O + \max(0, \eta-1)\ (x + y/4 - z/2)\ O_2 + \eta\ (x + y/4 - z/2)\ 3.76N_2$ (13)

For a methanol-air flame, Eq. (13) becomes:

$CH_3OH + 3/2\eta\ (O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)CH_3OH + \min(1, \eta)CO_2 + 2\min(1, \eta)H_2O + 3/2\max(0, \eta-1)\ O_2 + 5.64\eta\ N_2$ (14)

The mass fraction, Y_i, of products can be determined through the right side of Eq. (14) as follows:

$$Y_{CH_3OH} = \max(0,1-\eta)W_{CH_3OH} / W_{tot} \quad (15a)$$

$$Y_{CO_2} = \min(1,\eta)W_{CO_2} / W_{tot} \quad (15b)$$

$$Y_{H_2O} = 2\min(1,\eta)W_{H_2O} / W_{tot} \quad (15c)$$

$$Y_{O_2} = 3/2\max(0,\eta-1)W_{O_2} / W_{tot} \quad (15d)$$

$$Y_{N_2} = 5.64\eta W_{N_2} / W_{tot} \quad (15e)$$

Again, Y_{CO} and Y_{soot} in Eq. (1) were taken as zero.

The total molecular weight (W_{tot}) is a function of the local composition and was calculated from the reactant concentrations:

$$W_{tot} = W_{CH_3OH} + 3/2\eta(W_{O_2} + 3.76W_{N_2}) \quad (16)$$

Since Y_{CO} and Y_{soot} are assumed to be equal to zero and $Y_F = Y_{CH_3OH}$, Z in Eq. (1) is:

$$Z = Y_{CH_3OH} + Y_{CO_2}\frac{W_{CH_3OH}}{W_{CO_2}} \quad (17)$$

Putting in Eqs. (15) and (16), Z is:

$$Z = \frac{W_{CH_3OH}}{W_{tot}} = \frac{W_{CH_3OH}}{W_{CH_3OH} + 3/2\eta(W_{O_2} + 3.76W_{N_2})} \quad (18)$$

and η is:

$$\eta = \frac{1-Z}{Z}\frac{W_{CH_3OH}}{3/2(W_{O_2} + 3.76W_{N_2})} = \frac{1-Z}{Z}(F/A)_{st} \quad (19)$$

Relationships between Y_i and Z for methanol are plotted in Fig. 2.

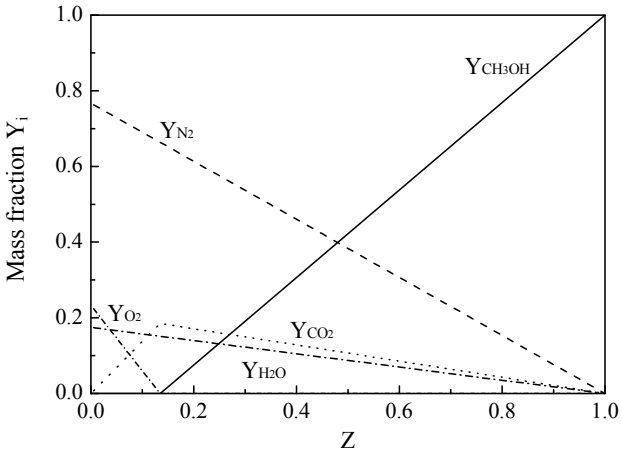

Fig. 2: State relations for methanol

5. ETHANOL

For ethanol, Eq. (13) becomes

$CH_3CH_2OH + 3\eta\ (O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)CH_3CH_2OH + 2\min(1,\eta)CO_2 + 3\min(1, \eta)H_2O + 3\max(0, \eta-1)\ O_2 + 11.28\eta\ N_2$ (20)

The mass fraction, Y_i, of products can be determined through the right side of Eq. (20) as follows:

$$Y_{CH_3CH_2OH} = \max(0,1-\eta)W_{CH_3CH_2OH} / W_{tot} \quad (21a)$$

$$Y_{CO_2} = 2\min(1,\eta)W_{CO_2} / W_{tot} \quad (21b)$$

$$Y_{H_2O} = 3\min(1,\eta)W_{H_2O} / W_{tot} \quad (21c)$$

$$Y_{O_2} = 3\max(0,\eta-1)W_{O_2} / W_{tot} \quad (21d)$$

$$Y_{N_2} = 11.28\eta W_{N_2} / W_{tot} \quad (21e)$$

The total molecular weight (W_{tot}) can be determined as follows:

$$W_{tot} = W_{CH_3CH_2OH} + 3\eta(W_{O_2} + 3.76W_{N_2}) \quad (22)$$

Z can be rewritten as:

$$Z = Y_{CH_3CH_2OH} + Y_{CO_2}\frac{W_{CH_3CH_2OH}}{2W_{CO_2}} \quad (23)$$

or

$$Z = \frac{W_{CH_3CH_2OH}}{W_{tot}} = \frac{W_{CH_3CH_2OH}}{W_{CH_3CH_2OH} + 3\eta(W_{O_2} + 3.76W_{N_2})} \quad (24)$$

Relationships between Y_i and Z for ethanol are plotted in Fig. 3.

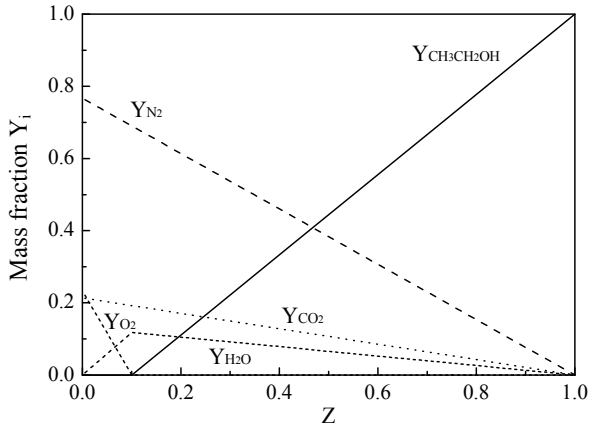

Fig. 3: State relations for ethanol

6. PROPANOL

For propanol (C_3H_8O), Eq. (13) becomes

$C_3H_8O + 9/2\eta\ (O_2 + 3.76N_2) \rightarrow \max(0, 1\text{-}\eta)C_3H_8O + 3\min(1, \eta)CO_2 + 4\min(1, \eta)H_2O + 9/2\max(0, \eta\text{-}1)\ O_2 + 16.92\eta\ N_2$ (25)

The mass fraction, Y_i, of products can be determined through the right side of Eq. (25) as follows:

$$Y_{C_3H_8O} = \max(0,1-\eta)W_{C_3H_8O} / W_{tot} \quad (26a)$$

$$Y_{CO_2} = 3\min(1,\eta)W_{CO_2} / W_{tot} \quad (26b)$$

$$Y_{H_2O} = 4\min(1,\eta)W_{H_2O} / W_{tot} \quad (26c)$$

$$Y_{O_2} = 4.5\max(0,\eta-1)W_{O_2} / W_{tot} \quad (26d)$$

$$Y_{N_2} = 16.92\eta W_{N_2} / W_{tot} \quad (26e)$$

The total molecular weight (W_{tot}) can be determined as follows:

$$W_{tot} = W_{C_3H_8O} + 4.5\eta(W_{O_2} + 3.76W_{N_2}) \quad (27)$$

Z can be rewritten as:

$$Z = Y_{C_3H_8O} + Y_{CO_2}\frac{W_{C_3H_8O}}{3W_{CO_2}} \quad (28)$$

or

$$Z = \frac{W_{C_3H_8O}}{W_{tot}} = \frac{W_{C_3H_8O}}{W_{C_3H_8O} + 4.5\eta(W_{O_2} + 3.76W_{N_2})} \quad (29)$$

Relationships between Y_i and Z for propanol are plotted in Fig. 4.

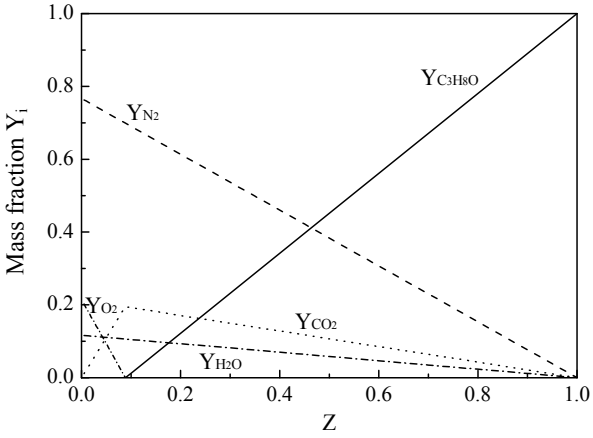

Fig. 4: State relations for propanol

7. GASOLINE

Gasoline is a mixture of hydrocarbons with octane (C_8H_{18}) considered as the main chemical compound. The octane number is therefore an important parameter to evaluate the performance of gasoline. Eq. (4) for gasoline becomes:

$C_8H_{18} + 12.5\eta(O_2 + 3.76N_2) \rightarrow \max(0, 1\text{-}\eta)\ C_8H_{18} + 8\min(1, \eta)\ CO_2 + 9\min(1, \eta)\ H_2O + 12.5\max(0, \eta\text{-}1)O_2 + 47\eta N_2$ (30)

The mass fraction, Y_i, of products can be determined through the right side of Eq. (30) as follows:

$$Y_{C_8H_{18}} = \max(0,1-\eta)W_{C_8H_{18}} / W_{tot} \quad (31a)$$

$$Y_{CO_2} = 8\min(1,\eta)W_{CO_2} / W_{tot} \quad (31b)$$

$$Y_{H_2O} = 9\min(1,\eta)W_{H_2O} / W_{tot} \quad (31c)$$

$$Y_{O_2} = 12.5\max(0,\eta-1)W_{O_2} / W_{tot} \quad (31d)$$

$$Y_{N_2} = 47\eta W_{N_2} / W_{tot} \quad (31e)$$

The total molecular weight (W_{tot}) can be determined as follows:

$$W_{tot} = W_{C_8H_{18}} + 12.5\eta(W_{O_2} + 3.76W_{N_2}) \quad (32)$$

Z can be rewritten as:

$$Z = Y_{C_8H_{18}} + Y_{CO_2}\frac{W_{C_8H_{18}}}{8W_{CO_2}} \quad (33)$$

or

$$Z = \frac{W_{C_8H_{18}}}{W_{tot}} = \frac{W_{C_8H_{18}}}{W_{C_8H_{18}} + 12.5\eta(W_{O_2} + 3.76W_{N_2})} \quad (34)$$

Relationships between Y_i and Z for gasoline are plotted in Fig. 5.

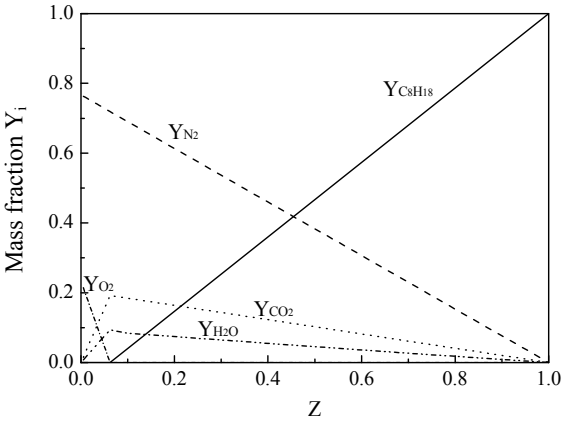

Fig. 5: State relations for gasoline

8. DIESEL

Diesel is a mixture of hydrocarbons with alkane ($C_{16}H_{34}$) considered as the main chemical compound. The alkane ($C_{16}H_{34}$) number is an important performance parameter of diesel and Eq. (4) becomes:

$$C_{16}H_{34} + 24.5\eta(O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)\, C_{16}H_{34} + 16\min(1, \eta)\, CO_2 + 17\min(1, \eta)\, H_2O + 24.5\max(0, \eta-1)O_2 + 92.12\eta N_2 \quad (35)$$

The mass fraction, Y_i, of products can be determined through the right side of Eq. (35) as follows:

$$Y_{C_{16}H_{34}} = \max(0,1-\eta)W_{C_{16}H_{34}} / W_{tot} \quad (36a)$$

$$Y_{CO_2} = 16\min(1,\eta)W_{CO_2} / W_{tot} \quad (36b)$$

$$Y_{H_2O} = 17\min(1,\eta)W_{H_2O} / W_{tot} \quad (36c)$$

$$Y_{O_2} = 24.5\max(0,\eta-1)W_{O_2} / W_{tot} \quad (36d)$$

$$Y_{N_2} = 92.12\eta W_{N_2} / W_{tot} \quad (36e)$$

The total molecular weight (W_{tot}) can be determined as follows:

$$W_{tot} = W_{C_{16}H_{34}} + 24.5\eta(W_{O_2} + 3.76W_{N_2}) \quad (37)$$

Z can be rewritten as:

$$Z = Y_{C_8H_{18}} + Y_{CO_2}\frac{W_{C_8H_{18}}}{16W_{CO_2}} \quad (38)$$

or

$$Z = \frac{W_{C_{16}H_{34}}}{W_{tot}} = \frac{W_{C_{16}H_{34}}}{W_{C_{16}H_{34}} + 24.5\eta(W_{O_2} + 3.76W_{N_2})} \quad (39)$$

Relationships between Y_i and Z for diesel are plotted in Fig. 6.

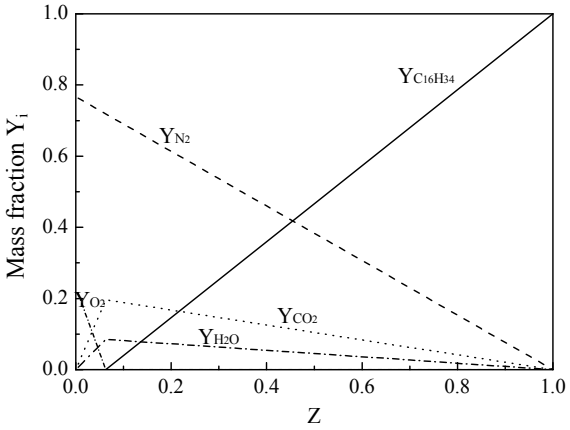

Fig. 6: State relations for diesel

9. POLYMETHYL METHACRYLATE

Polymethyl methacrylate (PMMA) $(C_5H_8O_2)_n$ is a thermoplastic polymer with monomer $C_5H_8O_2$. Therefore, Eq. (13) for PMMA becomes:

$$C_5H_8O_2 + 6\eta\,(O_2 + 3.76N_2) \rightarrow \max(0, 1-\eta)C_5H_8O_2 + 5\min(1, \eta)CO_2 + 4\min(1, \eta)H_2O + 6\max(0, \eta-1)\, O_2 + 22.56\eta\, N_2 \quad (40)$$

The mass fraction, Y_i, of products can be determined through the right side of Eq. (40) as follows:

$$Y_{C_5H_8O_2} = \max(0,1-\eta)W_{C_5H_8O_2} / W_{tot} \quad (41a)$$

$$Y_{CO_2} = 5\min(1,\eta)W_{CO_2} / W_{tot} \quad (41b)$$

$$Y_{H_2O} = 4\min(1,\eta)W_{H_2O} / W_{tot} \quad (41c)$$

$$Y_{O_2} = 6\max(0,\eta-1)W_{O_2} / W_{tot} \quad (41d)$$

$$Y_{N_2} = 22.56\eta W_{N_2} / W_{tot} \quad (41e)$$

The total molecular weight (W_{tot}) can be determined as follows:

$$W_{tot} = W_{C_5H_8O_2} + 6\eta(W_{O_2} + 3.76W_{N_2}) \quad (42)$$

Z can be rewritten as:

$$Z = Y_{C_5H_8O_2} + Y_{CO_2}\frac{W_{C_5H_8O_2}}{5W_{CO_2}} \quad (43)$$

or

$$Z = \frac{W_{C_5H_8O_2}}{W_{tot}} = \frac{W_{C_5H_8O_2}}{W_{C_5H_8O_2} + 6\eta(W_{O_2} + 3.76W_{N_2})} \quad (44)$$

Relationships between Y_i and Z for PMMA are plotted in Fig. 7.

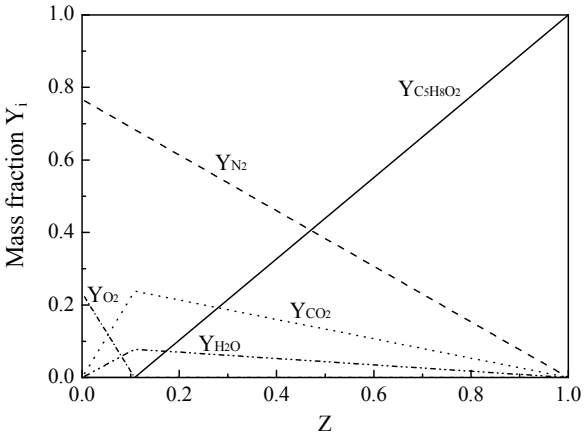

Fig. 7: State relations for PMMA

10. CONCLUSIONS

The method of mixture fraction in modeling combustion process in simulating building fires is reported. State relation is the key part and should be studied properly. The state relations of common fuels including methane, methanol, ethanol, propanol, gasoline, diesel and PMMA are estimated and reported. Results are useful in applying CFD-FDS in simulating heat release rate for hazard assessment. Predictions would be compared with experiments on gasoline pool fires, diesel pool fires and PMMA crib fires carried out in an oxygen consumption calorimeter. All these will be reported in later articles.

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