

Adiabatic Flame Temperature and Specific Heat of Combustion Gases

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Abstract

The aim of the present work is to examine adiabatic flame temperature and the specific heat of combustion gases for both hydrocarbon-air and alcohol-air mixtures by means of a method of chemical equilibrium calculation. Emphasis is placed on the elucidation of simplified correlation equations capable of predicting (i) adiabatic flame temperature at any equivalence ratio and (ii) the specific heat of combustion gases when the adiabatic flame temperature, the gas temperature and the equivalence ratio are varied. It was found that the detailed properties of combustion gas compositions, to a certain degree, can be predicted by the approximated equations, which, based on the results of the chemical equilibrium calculations, are produced with the aid of the method of least squares.

1. INTRODUCTION

Over the past few decades, the performance estimation of internal combustion engines has been made based on a knowledge of adiabatic flame temperature and equilibrium combustion gas composition. The information is very important in design and scale-up procedures wherever heat transfer is a significant consideration. NO_x formation in the internal combustion engines is studied by many investigators, and is mainly evaluated by means of chemical equilibrium calculation, which is one of the important methods for studying NO_x formation. In calculating heat release in internal combustion engines, specific heats of the combustion gases which are represented as functions of equivalence ratio and combustion gas temperature, must be obtained and the estimation accuracy of heat release is strongly effected on the specific heat. If two parameters are varied, the equilibrium combustion gas compositions need to be re-evaluated with the aid of a method of chemical equilibrium calculation.

The calculation of equilibrium flame gas composition was extremely time-consuming due to complexity of non-linear plural simultaneous equations to be solved. Accordingly, the corresponding tables and figures has been so far employed to evaluate this value, because the manner is simpler. However its prediction accuracy is inferior to that with the use of a method of chemical equilibrium calculation. From a knowledge of the flame gas compositions, the calculation of equilibrium flame temperature is a relatively simple operation, though this requires the equilibrium constants for the dissociation reactions to be expressed as a function of temperature. For the purpose of improving a situation, i. e. complexity mentioned above, Harker¹⁾ discussed the equilibrium flame gas compositions of gas mixtures resulting from the constant pressure combustion of hydrocarbon-air mixtures and proposed a simplified method for calculation in which the equilibrium products consisting of 10 chemical species were assumed.

The proposed study is intended to examine adiabatic flame temperature and specific heat of

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combustion gases for both hydrocarbon-air and alcohol-air mixtures by using a method of chemical equilibrium calculation and to evaluate two values with equivalence ratio as the parameter. The main object of the present work, based on the results, is to describe a simplified correlation equation of specific heat of the combustion gas when adiabatic flame temperature, gas temperature and equivalence ratio are varied. Results will be useful in the performance calculation of internal combustion engines.

2. CALCULATION METHOD

2.1 Basic Equations

Prior to the calculation of the equilibrium composition of flame gases in internal combustion engines, some assumptions are made as follows :

- (a) The flow is steady and one dimensional along the flame axis ;
- (b) The combustion products are homogeneous and its composition is constant throughout the flame;
- (c) The combustion products obey the ideal gas laws in the temperature range of 2500 to 4000 K ; and
- (d) The flow is adiabatic and isentropic.

When hydrocarbon fuels and alcohol are burnt with air, the gas mixture contains carbon, hydrogen, oxygen and nitrogen in the range of the flame temperature assumed above. The dissociation equilibrium which then have to be considered are :



and the following relationships must be satisfied under the condition of equilibrium.

$$K_1 = P_{\text{CO}} P_{\text{O}_2}^{0.5} / P_{\text{CO}_2} \quad (7)$$

$$K_2 = P_{\text{H}_2} P_{\text{O}_2}^{0.5} / P_{\text{H}_2\text{O}} \quad (8)$$

$$K_3 = P_{\text{OH}} P_{\text{H}_2}^{0.5} / P_{\text{H}_2\text{O}} \quad (9)$$

$$K_4 = P_{\text{H}} / P_{\text{H}_2}^{0.5} \quad (10)$$

$$K_5 = P_{\text{O}} / P_{\text{O}_2}^{0.5} \quad (11)$$

$$K_6 = P_{\text{NO}} / (P_{\text{O}_2}^{0.5} P_{\text{N}_2}^{0.5}) \quad (12)$$

where K_1 to K_6 are the equilibrium constants, which are a function of the gas temperature. By using $a = P_{\text{CO}}$, $b = P_{\text{CO}_2}$, etc. as given in the nomenclature, the partial pressures of O_2 , N_2 , etc. in Eqs. (7) to (12) and the total pressure, P , are described by the following relationship,

$$a + b + c + d + e + f + g + h + i + j = P, \quad (13)$$

and the equilibrium equations of (7) to (12) then are represented :

$$K_1 = ac^{0.5}/b \quad (14)$$

$$K_2 = dc^{0.5}/e \quad (15)$$

$$K_3 = fd^{0.5}/e \quad (16)$$

$$K_4 = g/d^{0.5} \quad (17)$$

$$K_5 = h/c^{0.5} \quad (18)$$

$$K_6 = i/(c^{0.5}j^{0.5}) \quad (19)$$

A further three equations may be obtained from the principle of mass balance :

$$\text{for carbon, } n_c = P_{\text{CO}} + P_{\text{CO}_2} = a + b \quad (20)$$

$$\text{for hydrogen, } n=2d+2e+f+g \quad (21)$$

$$\text{for oxygen, } n_o=a+2b+2c+e+f+h+i \quad (22)$$

$$\text{for nitrogen, } n_N=i+2j \quad (23)$$

Atomic numbers of n_c , n etc., are not known as absolute values, but their ratios can be obtained from a knowledge of the composition of the fuel-air mixture. Thus if $k=n_c/n$, $l=n_o/n$ and $m=n_N/n$, Eqs. (20) - (23) become :

$$kn=a+b \quad (24)$$

$$ln=a+2b+2c+e+f+h+i \quad (25)$$

$$mn=i+2j \quad (26)$$

$$n=2d+2e+f+g \quad (27)$$

Thus there are 11 equations and 11 unknowns, although a complete solution is impossible in that all equations can not be expressed in a linear form. In order to obtain a solution, the above equations are transformed into a more convenience form such as the relationship giving e as a function of d .

From Eq. (15),

$$c=e^2K_2/d^2 \quad (28)$$

Substituting Eq. (28) into Eq. (14), the form a is obtained.

$$a=bK_1d/eK_2 \quad (29)$$

Equations (16) and (17) are transformed into the following equations :

$$f=eK_3/d^{0.5}, \quad (30)$$

$$g=K_4d^{0.5}. \quad (31)$$

Partial pressure of h can be evaluated from Eqs. (18) and (28).

$$h=K_2K_5e/d \quad (32)$$

If Eqs. (28), (29), (30) and (32) are substituted for c , a , f and h , respectively, then Eq. (25) becomes:

$$i=ln-bK_1b/eK_2-2b-2e^2K_2/d^2-e-eK_3/d^{0.5}-K_2K_5e/d. \quad (33)$$

Substituting Eqs. (28), (29), (30), (31), (32) and (33) into Eq. (13), j is given by the following equation.

$$j=P+b+e^2K_2/d^2-d-K_4d^{0.5}-ln \quad (34)$$

Partial pressure of n can be evaluated submitting Eqs. (30) and (31) into Eq. (27).

$$n=2d+2e+eK_3/d^{0.5}+K_4d^{0.5} \quad (35)$$

Eqs. (29) and (35) are submitted into Eq. (24), resulting in the following equation for b :

$$b=[eK_2/(K_1d+K_2e)](2d+2e+eK_3/d^{0.5}+K_4d^{0.5}) \quad (36)$$

Finally e can be obtained by submitting Eq. (36) into Eq. (26).

$$e=(-Y+(Y^2-4XZ)^{0.5})/2X \quad (37)$$

where

$$X=K_2(2l+2m+1)+K_2K_3(l+m+1)/d^{0.5}+K_2^2K_5/d \quad (38)$$

$$Y=K_1d(2k+2l+2m+1)+2K_2d(l+m+1)+K_1K_3d^{0.5}(k+l+m+1)+K_2K_4d^{0.5}(l+m+2)+K_1K_2K_5-2PK_2 \quad (39)$$

$$Z=2K_1d^2(k+l+m+1)+K_1K_4dd^{0.5}(k+l+m+2)-2PK_1d \quad (40)$$

2.2 Calculation Process of Combustion Gas Composition

The calculations involve the simultaneous solution of both linear and non-linear algebraic equations, as mentioned before. Thus a solution is usually derived by means of trial and error methods. The combustion gas composition, if the combustion gas temperature T_b is given, can be obtained in the following process :

(a) Calculate k , l , and m corresponding to compositions of the fuel-air mixture ;

- (b) Assume a low value of d , for example $d=0.001$ P ;
- (c) Evaluate e from Eq. (37) using known values of K_i to K_e at T_b and k , l and m obtained above ;
- (d) Calculate the values of a , b , c , f , g , h , i and j from Eqs. (28) - (36) ;
- (e) Calculate the value ($=y$) of $K_e j^{0.5} c^{0.5}$ from Eq. (19) ; and
- (f) If $y \neq i$, a small increment x is added to d and the calculation repeats until $y=i$.

2.3 Calculation Process of Adiabatic Flame Temperature

For the calculation of the combustion gas composition and the adiabatic flame temperature T_b , the steps, if the composition and initial condition of the fuel-air mixture are given, are as follows :

- (a) Calculate enthalpy H_u , and values of k , l and m per 1 mole of the fuel-air mixture ;
- (b) Assume T_b ;
- (c) Estimate the combustion gas composition at T_b in the same manner as the previous section ;
- (d) Calculate enthalpy h_p and specific heat c_p corresponding to combustion gas ; and
- (e) if $h_b \neq H_u$, a small increment $(H_u - h_b)/c_p$ is added to T_b and the calculation repeats until $h_b = H_u$.

2.4 Calculation of Combustion Gas Properties

Specific heat c_p of the pure gas can be approximated as follows :

$T > 1200$ K

$$c_p = a_1 + a_2/\theta + a_3/\theta^2 + a_4/\theta^3 + a_5/\theta^4 \quad (41)$$

$T < 1200$ K

$$c_p = a_6 + a_7/\theta + a_8/\theta^2 + a_9/\theta^3 + a_{10}/\theta^4 \quad (42)$$

where $\theta = T/1000$,

Enthalpy h can be calculated by using the relationship :

$$h = c_p dT + h_{1200} = 1000 c_p d\theta + h_{1200} \quad (43)$$

Thus submitting Eq. (41) or (42) into Eq. (43), h is given :

$T > 1200$ K

$$h = a_{11} + 1000 (a_1 \theta + a_2 \ln \theta - a_3/\theta - \frac{1}{2} a_4/\theta^2 - \frac{1}{3} a_5/\theta^3) \quad (44)$$

$T < 1200$ K

$$h = a_{13} + 1000 (a_6 \theta + \frac{1}{2} a_7/\theta^2 + \frac{1}{3} a_8/\theta^3 + \frac{1}{4} a_9/\theta^4 + \frac{1}{5} a_{10}/\theta^5) \quad (45)$$

Entropy s , for constant pressure process, can be calculated from the following equation.

$$s = \int_{1200}^T c_p/T dT + s_{1200} = \int_{1,2}^{\theta} c_p/\theta d\theta + s_{1200} \quad (46)$$

By using Eqs. (41) and (42), a further transformation is made for Eq. (46).

$T > 1200$

$$s = a_{12} + a_1 \ln \theta - a_2/\theta - \frac{1}{2} a_3/\theta^2 - \frac{1}{3} a_4/\theta^3 - \frac{1}{4} a_5/\theta^4 \quad (47)$$

$T < 1200$

$$s = a_{14} + a_6 \ln \theta + a_7/\theta - \frac{1}{2} a_8/\theta^2 + \frac{1}{3} a_9/\theta^3 + \frac{1}{4} a_{10}/\theta^4 \quad (48)$$

Based on the thermochemical tables²⁾, the values of a_1 to a_{14} in the above equations were evaluated by means of the method of least squares. If specific heat, enthalpy and entropy for each composition are obtained, the corresponding values for the combustion gas can be calculated by the use of the relationships :

Table 1 Standard enthalpy of formation for each gas

fuel		$\Delta H_{f, 298}^{\circ}$ (cal/mol)
methanol	CH ₃ OH	-48108
ethanol	C ₂ H ₅ OH	-56279
methane	CH ₄	-17895
ethane	C ₂ H ₆	-20236
propane	C ₃ H ₈	-24820
hexane	n-C ₆ H ₁₄	-39950
octane	C ₈ H ₁₈	-49820
ethylene	C ₂ H ₄	+12540
propylene	C ₃ H ₆	+48790
acetylene	C ₂ H ₂	+54190
butane	n-C ₄ H ₁₀	-30150
decane	C ₁₀ H ₂₂	-59670

$$c_p = (c_{pCO}P_{CO} + c_{pCO_2}P_{CO_2} + c_{pO_2}P_{O_2} + c_{pH_2}P_{H_2} + c_{pH_2O}P_{H_2O} + c_{pOH}P_{OH} + c_{pH}P_H + c_{pO}P_O + c_{pNO}P_{NO} + c_{pN_2}P_{N_2})/P \quad (49)$$

$$h_b = (h_{CO}P_{CO} + h_{CO_2}P_{CO_2} + h_{O_2}P_{O_2} + h_{H_2}P_{H_2} + h_{H_2O}P_{H_2O} + h_{OH}P_{OH} + h_HP_H + h_OP_O + h_{NO}P_{NO} + h_{N_2}P_{N_2})/P \quad (50)$$

$$s = (s_{CO}P_{CO} + s_{CO_2}P_{CO_2} + s_{O_2}P_{O_2} + s_{H_2}P_{H_2} + s_{H_2O}P_{H_2O} + s_{OH}P_{OH} + s_HP_H + s_OP_O + s_{NO}P_{NO} + s_{N_2}P_{N_2})/P \quad (51)$$

In transforming enthalpy per 1 mole of the fuel-air mixture into that per 1 mole of the combustion gas, the following relationship is employed :

$$H_u = n_e / (n_d P). \quad (52)$$

The average molecular number M of the combustion gas is given by

$$M = (M_{CO}P_{CO} + M_{CO_2}P_{CO_2} + M_{O_2}P_{O_2} + M_{H_2}P_{H_2} + M_{H_2O}P_{H_2O} + M_{OH}P_{OH} + M_HP_H + M_OP_O + M_{NO}P_{NO} + M_{N_2}P_{N_2})/P \quad (53)$$

The equilibrium constants defined in Eqs. (14) to (19) can be obtained from the following equations in which the equilibrium constant for each gas is estimated by using the thermochemical tables²⁾.

$$\log_{10} K_1 = \log_{10} K_{CO} + 0.5 \log_{10} K_{O_2} - \log_{10} K_{CO_2} \quad (54)$$

$$\log_{10} K_2 = 0.5 \log_{10} K_{H_2} + 0.5 \log_{10} K_{O_2} - \log_{10} K_{H_2O} \quad (55)$$

$$\log_{10} K_3 = 0.5 \log_{10} K_{H_2} + \log_{10} K_{OH} - \log_{10} K_{H_2O} \quad (56)$$

$$\log_{10} K_4 = \log_{10} K_H - 0.5 \log_{10} K_{H_2} \quad (57)$$

$$\log_{10} K_5 = \log_{10} K_O - 0.5 \log_{10} K_{O_2} \quad (58)$$

$$\log_{10} K_6 = \log_{10} K_{NO} - 0.5 \log_{10} K_{O_2} - 0.5 \log_{10} K_{N_2} \quad (59)$$

where

$$K_{O_2} = K_{H_2} = K_{N_2} = 1. \quad (60)$$

These relationships are independent of temperature, because O₂, H₂ and N₂ are the fundamental gases.

2.5 Standard Enthalpy of Formation

The standard enthalpies of formation for the combustion gases were evaluated based on the thermochemical tables²⁾. The corresponding values of alcohol-fuels (methanol and ethanol) are calculated from the relationship between the heat of formation of alcohol and standard enthalpies of formation for CO₂ and H₂O³⁾ :

$$\Delta H_{f, 298}^{\circ} (C_xH_yO_z) = \Delta H_{f, 298}^{\circ} (C_xH_yO_z) + x \Delta H_{f, 298}^{\circ} (CO_2) + y/2 \Delta H_{f, 298}^{\circ} (H_2O) \quad (61)$$

Standard enthalpy of formation obtained for each gas is summarized in Table 1.

3. RESULTS AND DISCUSSION

3.1 Adiabatic Flame Temperature

For the adiabatic flame temperature of each fuel-air mixtures under the conditions of 1 atm and 298

K, the corresponding precise values were calculated by means of a method of the chemical equilibrium calculation. The results of methanol, ethanol, methane, ethane, propane, hexane, octane, ethylene, propylene, acetylene, butane and decane are represented in the form of adiabatic flame temperature versus equivalence ratio in Figs. 1 (a) to (l), respectively.

An attempt, based on the results, was made to derive a correlation equation capable of predicting adiabatic flame temperature at any equivalence ratio by means of the method of least squares. Elev-

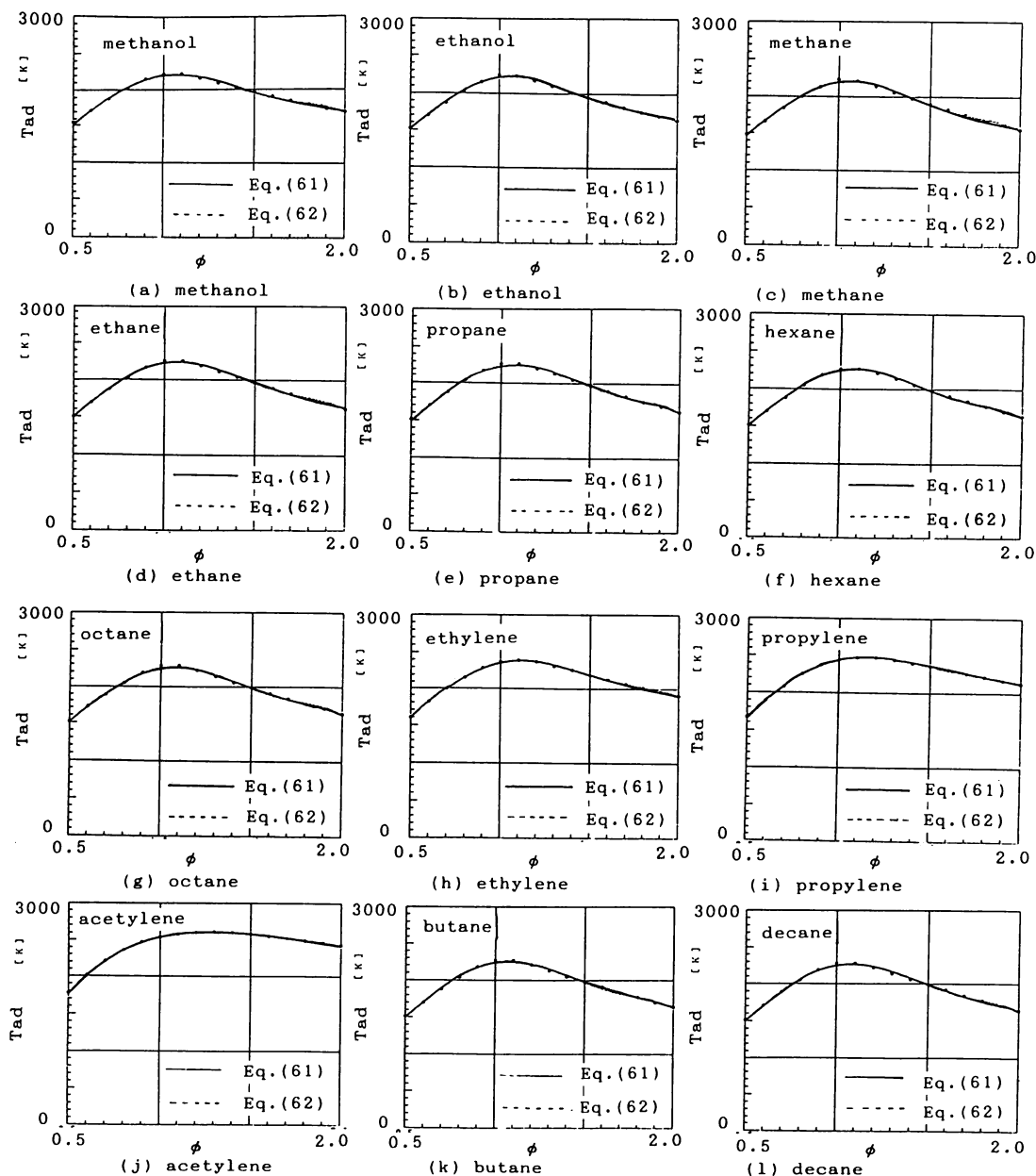


Fig. 1 Adiabatic flame temperature

enth and twelfth dimensional equations as the simpler equations were applied here :

$$T_{ad} = A_0 + A_1 \phi + A_2 \phi^2 + \dots + A_6 \phi^6 + A_7 \phi^7 \quad (61)$$

$$T_{ad} = A_0 + A_1 \phi + A_2 \phi^2 + \dots + A_{11} \phi^{11} + A_{12} \phi^{12} \quad (62)$$

Equations (61) and (62) are superimposed on Figs. 1 (a) to (l) as solid and dotted lines, respectively. Coefficients in Eqs. (61) and (62), i. e. A_0 , A_1 , etc., are summarized in Table 2 and 3. Throughout the results, it is disclosed that : (1) Maximum adiabatic flame temterature for each gas becomes in the vicinity of $\phi = 1$ and the results can be supported also by Table 4, which is formed by means of a method of chemical equilibrium calculation ; (2) Acetylene is the highest adiabatic flame temperature whose equivalence ratio is 1.3 ; (3) Alcohol fuels (methanol and ethanol) show the relatively low temperature than hydrocarbon fuels ; and (4) As expected, the prediction accuracy of Eq. (62) is superior to that of Eq. (61) for each equivalence ratio.

Table 2 Coefficients of 7 th dimensional correlation

fuel	A_0	A_1	A_2	A_3	A_4	A_5	A_6	A_7
methanol	1010.10	-561.210	4470.69	-1871.18	-1660.30	426.150	575.714	-195.582
ethanol	1049.20	-932.221	5070.42	-1975.08	-1896.05	465.822	641.356	-216.014
methane	1181.03	-1682.86	6050.05	-2131.45	-2234.57	496.133	760.695	-251.725
ethane	1112.33	-1340.76	5682.78	-2080.42	-2107.45	486.239	712.290	-236.978
propane	1101.44	-1290.67	5655.17	-2129.82	-2028.4	451.636	713.503	-235.487
hexane	1095.06	-1254.77	5622.99	-2135.01	-1999.66	439.898	710.795	-233.926
octane	1087.08	-1227.57	5607.62	-2139.13	-2019.47	483.263	684.855	-228.927
ethylene	760.196	468.383	3567.05	-1827.17	-1320.52	442.143	418.099	-150.217
propylene	393.638	2278.44	1378.00	-1488.84	-587.809	366.664	173.595	-77.0859
acetylene	-189.332	5055.66	-1891.93	-1067.31	507.129	301.619	-208.286	32.6057
butane	1099.96	-1272.84	5601.41	-2039.07	-2104.76	484.454	706.445	-234.866
decane	1078.96	-1175.33	5488.12	-2007.05	-2084.27	488.345	690.995	-230.431

Table 3 Coefficients of 12 th dimensional correlation

fuel	A_0	A_1	A_2	A_3	A_4	A_5	A_6	A_7
methanol	2116.51	-4985.65	9773.85	-3145.16	-2272.71	116.324	389.412	254.626
ethanol	2230.81	-5648.11	10716.8	-3363.14	-2482.08	119.842	409.363	276.604
methane	2666.44	-7642.73	13263.5	-3972.18	-3037.22	142.580	504.756	325.975
ethane	2410.28	-6531.19	11930.0	-3668.29	-2729.55	121.985	452.311	299.385
propane	2351.20	-6268.32	11584.3	-3538.81	-2680.21	102.528	447.182	293.684
hexane	2319.11	-6125.09	11410.4	-3490.32	-2643.63	91.1660	449.109	289.701
octane	2275.54	-5953.39	11224.9	-3484.38	-2581.53	105.408	427.814	286.742
ethylene	1397.16	-2025.52	6424.51	-2407.37	-1525.91	86.2291	254.085	196.337
propylene	639.481	1343.58	2366.18	-1605.76	-572.852	71.1606	108.255	118.910
acetylene	-140.717	4879.00	-1803.64	-793.321	283.791	117.020	-0.984833	30.0932
butane	2346.17	-6255.99	11604.1	-3592.27	-2652.70	113.245	438.373	295.718
decane	2271.66	-5936.86	11209.1	-3482.94	-2583.82	118.611	420.461	285.547

Table 3 Coefficients of 12 th dimensional correlation

fuel	A ₈	A ₉	A ₁₀	A ₁₁	A ₁₂
methanol	51.4397	-66.5194	-26.9156	-1.86958	5.62146
ethanol	60.5032	-71.8141	-29.5445	-2.30006	6.16903
methane	72.7182	-86.6642	-35.2819	-2.74363	7.42652
ethane	65.6856	-77.0223	-32.4034	-2.74673	6.79536
propane	67.0311	-76.5654	-32.2738	-2.29236	6.58517
hexane	63.7954	-75.1058	-31.5766	-2.21915	6.44869
octane	62.8623	-73.4601	-30.8627	-2.35395	6.35834
ethylene	29.1840	-46.7999	-17.2719	-1.42665	3.78032
propylene	0.829639	-23.8180	-6.32315	-0.955054	1.79099
acetylene	-31.9044	-2.83132	-4.76981	-0.47436	0.00000
butane	64.1072	-76.4019	-31.0823	-2.60731	6.57058
decane	63.5728	-73.4099	-30.3716	-2.67058	6.40715

Table 4 Maximum adiabatic flame temperature for each gas

fuel	adiabatic flame temperature [K]	equivalence ratio
methanol	2221.05	1.0
ethanol	2236.29	1.0
methane	2225.43	1.0
ethane	2258.88	1.0
propane	2266.54	1.0
butane	2269.20	1.0
hexane	2273.74	1.1
octane	2276.09	1.1
decane	2278.06	1.1
ethylene	2392.01	1.1
propylene	2473.37	1.1
acetylene	2607.57	1.3

3.2 Specific Heat of Combustion Gas

By using the calculation process mentioned in the previous section, which estimates the equilibrium combustion gas composition and the properties of the combustion gas if the combustion temperature is given, specific heats for methanol, ethanol, methane and propane were obtained under the condition of 1 atm and 298 K. The results obtained are illustrated in Figs. 2 to 5 with solid circle in which (a) and (b) correspond to specific heat and molar heat at constant pressure, respectively.

An attempt was made to derive an simpler equation capable of correlating specific heat and molar heat in the same manner as the previous section. Sixth and eighth dimensional equations were applied for specific heat and molar heat, respectively :

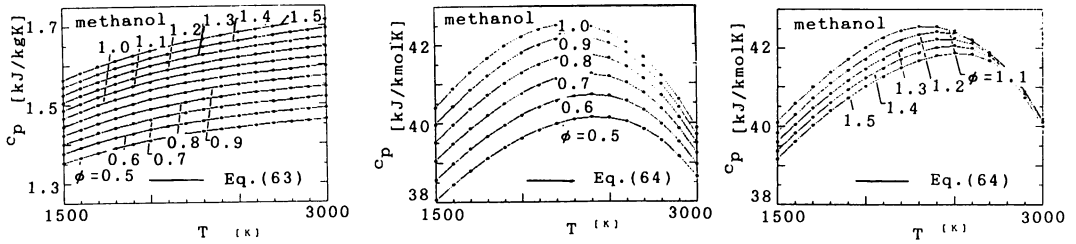
specific heat at constant pressure [kJ/kgK]

$$c_p = A_0 + A_1 \theta + A_2 \theta^2 + \cdots + A_5 \theta^5 + A_6 \theta^6 \quad (63)$$

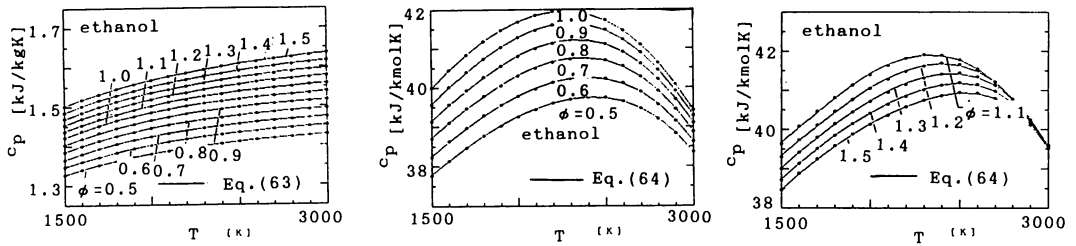
molar heat at constant pressure [kJ/kmolK]

$$c_p = A_0 + A_1 \theta + A_2 \theta^2 + \cdots + A_7 \theta^7 + A_8 \theta^8 \quad (64)$$

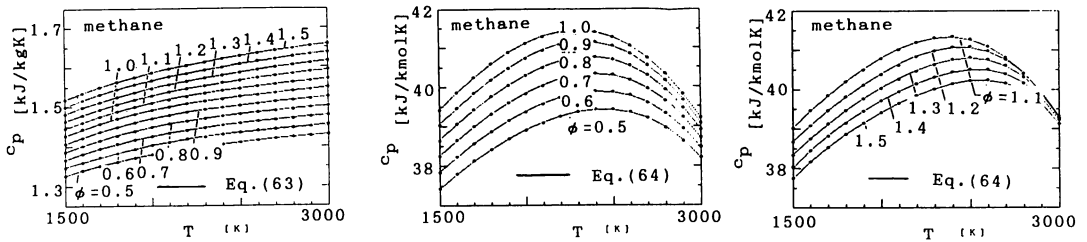
Equations (63) and (64) are depicted in figures as solid carved lines. Coefficients in Eqs. (63) and (64)



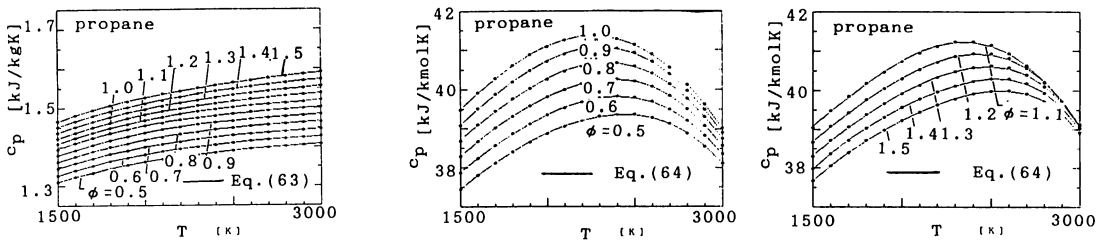
(a) Specific heat at constant pressure (b) Molar heat at constant pressure
Fig. 2 Methanol



(a) Specific heat at constant pressure (b) Molar heat at constant pressure
Fig. 3 Ethanol



(a) Specific heat at constant pressure (b) Molar heat at constant pressure
Fig. 4 Methane



(a) Specific heat at constant pressure (b) Molar heat at constant pressure
Fig. 5 Propane

are summarized in Tables 5 (a) and (b) for methanol, Tables 6 (a) and (b) for ethanol, Tables 7 (a) and (b) for methane and Tables 8 (a) and (b) for propane. Specific heat at constant pressure is increased in proportion to combustion temperature and/or equivalence ratio, and methanol shows a relatively high value than the other fuels. In contrast, a variation of molar heat at constant pressure, if

Table 5 Coefficients of correlation (methanol)
(a) Specific heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄	A ₅	A ₆
0.5	0.982757	0.335255	-3.98512 E -02	-1.71395 E -02	8.59580 E -04	1.77197 E -04	-2.81030 E -04
0.6	0.904921	0.479914	-1.06502 E -01	-5.48024 E -03	-1.70310 E -03	3.22731 E -03	-5.40113 E -04
0.7	1.163880	0.085917	1.14752 E -01	-5.20575 E -02	4.69883 E -03	1.12129 E -04	8.57008 E -05
0.8	1.041770	0.298186	1.38384 E -02	-3.54391 E -02	2.34061 E -03	1.74527 E -03	-2.35896 E -04
0.9	0.959344	0.478344	-1.09485 E -02	1.03911 E -02	-8.47949 E -03	3.51530 E -03	-3.91189 E -04
1.0	1.103690	0.242212	5.76083 E -02	-4.52607 E -02	2.92925 E -03	1.21215 E -03	-8.35839 E -05
1.1	1.063460	0.353939	-2.14028 E -02	-1.85742 E -02	-2.27271 E -03	2.23847 E -03	-2.31638 E -04
1.2	1.072600	0.370433	-2.55162 E -02	-2.38632 E -02	9.65527 E -04	1.79291 E -03	-2.43615 E -04
1.3	1.033850	0.451012	-5.65916 E -02	-2.12088 E -02	-1.89308 E -03	4.01015 E -03	-6.26210 E -04
1.4	1.099940	0.379289	-2.09959 E -02	-2.83551 E -02	3.78035 E -04	2.86965 E -03	-4.36869 E -04
1.5	1.106620	0.365263	1.98529 E -02	-5.02011 E -02	1.13936 E -03	4.85053 E -03	-7.97874 E -04

(b) Molar heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄
0.5	24.0735	1.53197 E +01	-3.63910 E +00	-8.86657 E -01	3.39202 E -01
0.6	27.9677	1.01357 E +01	-1.81969 E +00	-3.75773 E -01	8.57455 E -02
0.7	32.1662	4.46602 E +00	3.00950 E -01	-3.53402 E -02	-6.33871 E -02
0.8	35.0849	7.15039 E -01	1.60713 E +00	1.37306 E -01	3.80800 E -02
0.9	37.1389	-2.30203 E +00	3.10774 E +00	2.40243 E -01	-1.18643 E -01
1.0	30.3625	7.36888 E +00	3.09586 E -01	-4.86021 E -01	-6.59685 E -02
1.1	36.6754	-7.00143 E -02	1.12561 E +00	5.55257 E -01	2.67988 E -02
1.2	32.2909	6.07932 E +00	-9.42599 E -01	7.82267 E -02	1.00315 E -01
1.3	30.0211	8.45385 E +00	-1.08708 E +00	-4.31634 E -01	1.26300 E -01
1.4	28.2359	1.04416 E +01	-1.70478 E +00	-4.03873 E -01	8.03315 E -02
1.5	26.5216	1.21904 E +01	-2.05040 E +00	-4.96702 E -01	3.31503 E -02

equivalence ratio	A ₅	A ₆	A ₇	A ₈
0.5	1.27000 E -01	-2.84735 E -02	-1.45979 E -02	2.99467 E -03
0.6	8.29448 E -02	-1.74690 E -02	-8.66049 E -03	1.78078 E -03
0.7	-3.50133 E -04	2.39105 E -03	-4.71309 E -03	8.70681 E -04
0.8	-1.37477 E -01	-1.19254 E -04	1.15569 E -02	-1.64206 E -03
0.9	-1.61595 E -01	1.84132 E -02	9.46772 E -03	-1.55964 E -03
1.0	6.45887 E -02	-1.60716 E -02	-3.95718 E -03	1.18307 E -03
1.1	-1.35551 E -01	-2.23562 E -03	4.34445 E -03	2.00333 E -04
1.2	6.70702 E -03	-1.78217 E -02	-4.79069 E -03	1.46836 E -03
1.3	5.18997 E -02	-9.24711 E -03	-8.26054 E -03	1.24234 E -03
1.4	5.25206 E -02	-3.83899 E -03	-4.15293 E -03	-8.30914 E -05
1.5	7.82255 E -01	-5.68492 E -03	-9.87498 E -04	-9.85191 E -04

Table 6 Coefficients of correlation (ethanol)
(a) Specific heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄	A ₅	A ₆
0.5	1.043440	0.202113	3.41656 E -02	-3.59596 E -02	3.50745 E -03	1.21129 E -03	-1.86830 E -04
0.6	1.072040	0.191317	2.82023 E -02	-2.56999 E -02	1.29720 E -03	6.32435 E -04	-1.79267 E -05
0.7	0.939771	0.425046	-9.54696 E -02	2.09826 E -03	-3.98405 E -03	2.70001 E -03	-3.73437 E -04
0.8	0.880184	0.542662	-1.56242 E -01	1.48581 E -02	-5.22046 E -03	3.04882 E -03	-4.47196 E -04
0.9	1.032550	0.303846	-1.15847 E -02	-1.65699 E -02	-3.75195 E -03	2.49592 E -03	-2.44359 E -04
1.0	0.994195	0.366737	-1.55465 E -02	-3.40083 E -02	3.24469 E -03	1.80721 E -03	-2.75076 E -04
1.1	1.105450	0.245494	1.06254 E -02	-1.50267 E -02	-4.28533 E -03	1.79012 E -03	-8.43062 E -05
1.2	0.955745	0.525339	-1.48660 E -01	1.62697 E -02	-5.23565 E -03	2.59604 E -03	-3.59416 E -04
1.3	0.930939	0.550557	-1.18216 E -01	-1.04129 E -02	-3.16040 E -03	5.18034 E -03	-8.82210 E -04
1.4	0.976596	0.519798	-1.21391 E -01	1.74624 E -03	-6.48476 E -03	4.96361 E -03	-7.61091 E -04
1.5	0.995345	0.496169	-9.17504 E -02	-8.20409 E -03	-8.92528 E -03	6.96027 E -03	-1.05555 E -03

(b) Molar heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄
0.5	29.6446	6.70101 E +00	-9.71354 E -01	-4.64779 E -02	5.08430 E -02
0.6	31.3992	4.78580 E +00	1.52652 E -01	-1.44528 E -01	-4.95121 E -02
0.7	31.7295	5.08324 E +00	-2.31461 E -01	-1.47805 E -02	2.67727 E -02
0.8	31.405	6.02222 E +00	-5.11209 E -01	-6.94512 E -02	4.85149 E -02
0.9	32.357	4.58221 E +00	4.87263 E -01	-2.26511 E -01	6.62028 E -02
1.0	26.0429	1.39765 E +01	-2.79070 E +00	-5.64128 E -01	1.68926 E -01
1.1	39.8672	-5.28136 E +00	3.03869 E +00	8.26744 E -01	-1.26314 E -01
1.2	36.4832	-8.96282 E -01	1.99050 E +00	1.22988 E -01	-3.22035 E -02
1.3	32.8511	3.55931 E +00	7.29264 E -01	-1.92692 E -01	1.96918 E -03
1.4	27.3456	1.08909 E +01	-1.62473 E +00	-6.54715 E -01	7.43663 E -02
1.5	27.6691	9.36850 E +00	-4.07578 E -01	-8.59557 E -01	-3.53801 E -02

equivalence ratio	A ₅	A ₆	A ₇	A ₈
0.5	3.81642 E -03	-2.35568 E -02	7.84208 E -03	-1.02452 E -03
0.6	2.27660 E -02	-8.95386 E -03	-3.35475 E -04	1.73850 E -04
0.7	-9.82266 E -03	-1.55065 E -02	2.51858 E -03	6.14673 E -05
0.8	-5.67620 E -03	-2.93616 E -04	-8.73172 E -03	1.95996 E -03
0.9	-2.38038 E -02	-1.27018 E -02	-7.11896 E -04	9.36126 E -04
1.0	9.73767 E -02	-2.82970 E -02	-1.04269 E -02	2.72484 E -03
1.1	-2.15499 E -01	1.95540 E -02	1.09334 E -02	-1.48545 E -03
1.2	-8.17197 E -02	3.78255 E -03	3.52173 E -03	-5.27705 E -04
1.3	-2.30042 E -02	-5.87318 E -03	6.87593 E -03	-1.62184 E -03
1.4	9.16490 E -02	-2.70665 E -03	-8.26188 E -03	5.47284 E -04
1.5	1.06871 E -01	4.29777 E -03	-6.45122 E -03	-2.30570 E -04

Table 7 Coefficients of correlation (methane)
(a) Specific heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄	A ₅	A ₆
0.5	0.996344	0.276290	-4.71598 E -03	-2.81849 E -02	2.05674 E -03	1.97159 E -03	-3.25161 E -04
0.6	1.164190	0.016859	1.54259 E -01	-6.91916 E -02	9.04584 E -03	-2.27821 E -04	5.84365 E -05
0.7	1.005510	0.304774	-1.27567 E -02	-2.30108 E -02	-9.16510 E -04	2.59553 E -03	-3.59479 E -04
0.8	0.905864	0.505916	-1.343323 E -0	5.58381 E -03	-5.64759 E -04	1.47554 E -03	-2.42598 E -04
0.9	1.099620	0.191351	6.04350 E -02	-3.73598 E -02	-3.11729 E -04	1.83763 E -03	-1.44254 E -04
1.0	0.921978	0.507910	-1.15746 E -01	2.38377 E -03	-5.05009 E -03	3.32230 E -03	-4.37712 E -04
1.1	1.133230	0.195588	5.92718 E -02	-4.04392 E -02	3.46904 E -03	4.80325 E -04	1.54544 E -05
1.2	0.933854	0.560814	-1.55000 E -01	1.40770 E -02	-7.10227 E -03	4.15868 E -03	-6.09391 E -04
1.3	0.992584	0.469501	-7.06529 E -02	-2.61137 E -02	3.08388 E -03	2.94586 E -03	-5.63836 E -04
1.4	0.959005	0.568237	-1.44191 E -01	3.00983 E -03	-4.36175 E -03	4.34277 E -03	-7.02971 E -04
1.5	1.044700	0.449456	-6.46160 E -02	-2.52555 E -02	3.68795 E -03	2.26522 E -03	-4.38766 E -04

(b) Molar heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄
0.5	31.9889	2.65558 E +00	1.04294 E +00	-5.62901 E -02	-8.49118 E -02
0.6	28.3408	8.72547 E +00	-1.24558 E +00	-4.65472 E -01	1.25626 E -01
0.7	32.8185	2.38049 E +00	1.26660 E +00	-1.93818 E -01	1.57472 E -02
0.8	33.714	1.72255 E +00	1.20626 E +00	1.33211 E -01	-7.47731 E -02
0.9	37.8254	-4.04941 E +00	3.19866 E +00	6.97724 E -01	-2.16052 E -01
1.0	33.2229	2.17839 E +00	1.98884 E +00	-1.93385 E -01	-9.84355 E -02
1.1	28.5411	1.03850 E +01	-2.36646 E +00	-3.03501 E -01	2.23518 E -01
1.2	27.4636	1.12629 E +01	-2.30768 E +00	-5.93128 E -01	2.44557 E -01
1.3	27.7073	9.63764 E +00	-9.85230 E -01	-7.00649 E -01	4.15509 E -02
1.4	21.2557	1.83363 E +01	-3.95401 E +00	-1.15965 E +00	1.64036 E -01
1.5	26.4961	1.02370 E +01	-1.10389 E +00	-6.18502 E -01	3.08733 E -02

equivalence ratio	A ₅	A ₆	A ₇	A ₈
0.5	-7.08270 E -02	2.32765 E -02	2.81379 E -03	-1.31888 E -03
0.6	5.98091 E -02	-2.71769 E -02	4.98751 E -05	4.14303 E -04
0.7	-6.25935 E -02	-2.08352 E -03	7.66048 E -03	-1.32988 E -03
0.8	-6.85137 E -02	2.86890 E -03	5.16701 E -03	-7.78980 E -04
0.9	-2.24846 E -01	3.14323 E -02	1.64557 E -02	-3.19876 E -03
1.0	-7.44702 E -02	8.06728 E -03	7.02612 E -03	-1.28090 E -03
1.1	8.59454 E -02	-3.66226 E -02	-1.11881 E -02	3.23914 E -03
1.2	9.91830 E -02	-3.76515 E -02	-5.24024 E -03	1.49733 E -03
1.3	8.98160 E -02	1.68628 E -03	-9.75850 E -03	8.17572 E -04
1.4	2.28110 E -01	-2.29464 E -02	-1.65993 E -02	2.15773 E -03
1.5	2.82184 E -02	1.40812 E -02	-1.20025 E -03	-1.28855 E -03

Table 8 Coefficients of correlation (propane)
(a) Specific heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄	A ₅	A ₆
0.5	0.874505	0.477457	-1.43720 E -01	1.50602 E -02	-5.28791 E -03	3.20681 E -03	-4.98305 E -04
0.6	0.916491	0.417444	-9.49179 E -02	-1.61214 E -03	-2.45804 E -03	2.78417 E -03	-4.40599 E -04
0.7	0.966921	0.333140	-2.38684 E -02	-2.47473 E -02	-9.54672 E -04	3.39736 E -03	-5.28169 E -04
0.8	1.056570	0.234182	3.41594 E -03	-1.59135 E -02	-1.48073 E -03	9.98518 E -04	-2.32704 E -05
0.9	1.017270	0.293887	-1.58226 E -03	-2.70476 E -02	7.82845 E -04	1.71623 E -03	-2.06407 E -04
1.0	1.051300	0.249759	2.86809 E -02	-2.78687 E -02	-4.97525 E -03	3.63724 E -03	-3.89893 E -04
1.1	1.000240	0.389248	-7.70462 E -02	2.63363 E -04	-2.51157 E -03	1.39742 E -03	-1.33014 E -04
1.2	0.969036	0.464756	-1.19476 E -01	1.14169 E -02	-6.78625 E -03	3.39125 E -03	-4.55624 E -04
1.3	1.031970	0.377106	-6.02763 E -02	-6.36016 E -03	-5.03782 E -03	3.60065 E -03	-4.93285 E -04
1.4	1.103620	0.243339	6.25901 E -02	-6.13503 E -02	6.76816 E -03	2.71521 E -03	-5.13776 E -04
1.5	0.770988	0.824194	-2.83618 E -01	3.41828 E -02	-1.42034 E -02	9.13051 E -03	-1.49773 E -03

(b) Molar heat at constant pressure

equivalence ratio	A ₀	A ₁	A ₂	A ₃	A ₄
0.5	27.3475	9.93905 E +00	-1.90992 E +00	-3.99871 E -01	1.39354 E -01
0.6	29.8022	7.01682 E +00	-9.70942 E -01	-1.65486 E -01	5.69140 E -02
0.7	24.0648	1.58356 E +01	-3.87896 E +00	-9.40635 E -01	3.01414 E -01
0.8	32.7398	3.71969 E +00	1.78678 E -01	4.65098 E -02	6.09117 E -02
0.9	30.5971	7.13550 E +00	-1.13282 E +00	1.48224 E -01	-2.15756 E -02
1.0	34.7851	2.58209 E -01	2.39866 E +00	1.88942 E -01	-2.46129 E -01
1.1	36.982	-1.63019 E +00	1.76273 E +00	4.49680 E -01	-3.95758 E -03
1.2	32.4638	4.25597 E +00	3.85761 E -02	-1.15126 E -01	7.21795 E -02
1.3	27.6201	1.03626 E +01	-1.61877 E +00	-7.87948 E -01	2.45150 E -01
1.4	20.65	1.94307 E +01	-4.18192 E +00	-1.61329 E +00	3.14919 E -01
1.5	27.1385	9.33822 E +00	-6.70901 E -01	-7.09442 E -01	-3.76031 E -02

equivalence ratio	A ₅	A ₆	A ₇	A ₈
0.5	3.45675 E -02	-3.37652 E -03	-7.12367 E -03	1.11007 E -03
0.6	2.1601 E -02	-1.26096 E -02	-1.47042 E -03	5.08941 E -04
0.7	2.15517 E -01	-5.23617 E -02	-1.87929 E -02	4.54087 E -03
0.8	-6.33309 E -02	-8.34672 E -04	4.18792 E -05	4.52991 E -04
0.9	2.50249 E -02	-1.93232 E -02	-2.95694 E -03	1.42169 E -03
1.0	-1.16327 E -01	3.56920 E -02	2.51766 E -03	-9.96108 E -04
1.1	-1.23609 E -01	-1.28942 E -02	1.16518 E -02	-1.02495 E -03
1.2	-1.37261 E -02	-1.27753 E -02	1.93386 E -03	-1.20985 E -04
1.3	7.89523 E -02	-3.838137 E -0	3.88160 E -03	-5.08978 E -04
1.4	3.04176 E -01	-6.38027 E -02	-1.28737 E -02	2.51583 E -03
1.5	9.39212 E -02	-7.41617 E -03	1.40861 E -03	-1.29674 E -03

the combustion temperature is increased, is not somewhat different from that of specific heat mentioned above. For $\phi < 1.0$, molar heat is linearly increased with equivalence ratio, while the values, for $\phi > 1.0$, is decreased with an increase in equivalence ratio. The correlation equation predicts to a certain degree the data obtained by a method of chemical equilibrium calculation in the temperature range of 1500 to 3000 K.

4. SUMMARY

A method of chemical equilibrium calculation has been employed to evaluate adiabatic flame temperature and specific heat of combustion gases for both hydrocarbon-air and alcohol-air mixtures under the condition of 1 atm and 298 K. The results obtained are summarized as follows :

- (1) The adiabatic flame temperatures for hydrocarbon fuels are lower than those for alcohol fuels. The corresponding values can be predicted by the twelfth dimensional correlation equation, which is derived using the method of least squares.
- (2) Specific heat at constant pressure increases linearly with combustion gas temperature and/or equivalence ratio. Molar heat at constant pressure, for $\phi < 1.0$, varies with the same manner as specific heat, while for $\phi > 1.0$ the value decreases with increasing equivalence ratio. Specific and molar heats can be predicted to a certain degree by the sixth and eighth dimensional correlation equations, respectively.

NOMENCLATURE

a	partial pressure of CO
b	partial pressure of CO ₂
c	partial pressure of O ₂
c _p	specific heat
d	partial pressure of H ₂
e	partial pressure of H ₂ O
f	partial pressure of OH
g	partial pressure of H
h	partial pressure of O
h _b	enthalpy of combustion gas
H _a	enthalpy of fuel-air mixture
i	partial pressure of NO
j	partial pressure of N ₂
k	n _c /n
K ₁ -K ₆	equilibrium constants
l	n _o /n
n	amount of hydrogen in flame gases
n _c	amount of carbon in flame gases
n _o	amount of oxygen in flame gases
P	total pressure
s	entropy
T	gas temperature
X, Y, Z	functions of d
θ	T/1000

ϕ equivalence ratio

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