A new approach for simplifying the calculation of flue gas specific heat and specific exergy value depending on fuel composition

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ABSTRACT

In this paper, a new approach is proposed for simplifying the calculation of flue gas specific heat and specific exergy value in one formulation depending on fuel chemical composition. Combustion products contain different gases such as CO_2, SO_2, N_2, O_2, H_2O and etc., depending on the burning process. Specific heat and exergy of the flue gas differ depending on the chemical composition of fuels, excess air ratio and gas temperature. Through this new approach, specific heat and specific exergy value of combustion products can be estimated accurately in one formulation by entering the chemical composition of fuels, excess air ratio and gas temperature. The present approach can be applied to all carbon based fuels, especially biomass, fossil fuels and fuel mixtures for co-combustion and is so suitable for practical estimation of flue gas specific heat and specific exergy values provided that the fuel chemical composition is given.

1. Introduction

In general application, heat transfer surfaces of the boiler, economizer, heat exchanger, air heater and super heater are calculated depending on the flue gas enthalpy values. Flue gas enthalpy value is a function of specific heat and temperature. Chemical composition of fuel, excess air amount and gas temperature directly affect flue gas specific heat. Some researchers [1–5] investigated the effects of these parameters on combustion. Estimation of the flue gas real enthalpy values has a great effect on cost optimization. To make calculation by using the approximate values of flue gas causes two problems in design and operation. (i) When flue gas enthalpy values are considered lower than real values, system cost increases and (ii) existing heat transfer surface will not be sufficient when flue gas enthalpy values are taken higher. Engineers or designers face some difficulties in the process of the flue gas enthalpy value estimation. These difficulties may be explained in two parts; firstly, the graphics of flue gas enthalpies commonly used are drawn for only specific chemical composition of fuels. But the composition of the fuels is not the same every time. For instance, lignite coal compositions differ depending on the regions and mines. Enthalpy values of the combustion products can

be approximated employing these graphics given by many researchers [6–10]. Also, energy and exergy analysis of energy conservation process are investigated by many researchers [11–14]. Secondly, in literature, there exists enthalpy graphics for some well-known fossil fuels but not for biomass and fuel mixtures for co-combustion. Recently, the biomass and fuel mixtures for co-combustion have become more popular [15,16]. It is difficult to calculate and prepare the graphics for all fuels.

In this study, we present a new approach to achieve the accurate specific heat and exergy value. Through this new approach, specific heat and exergy value of combustion products can be estimated accurately in one formulation by entering the chemical composition of fuels, excess air ratio and gas temperature. In open literature, there is no formulation allowing the calculation of the specific heat and exergy values taking into account these three parameters.

2. Modeling

2.1. Balance equations

2.1.1. Mass balance

Theoretical combustion reaction for carbon, hydrogen and sulphur is given in the following equations [17].

$$C + (O_2 + 3.76\,N_2) \rightarrow CO_2 + 3.76\,N_2 \tag{1}$$
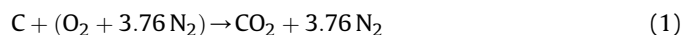
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Nomenclature		Subscripts	
		A	air
C_p	specific heat (kJ/kg K)	Ave.	average
h	enthalpy (kJ/kg-flue gas)	C	carbon
m	mass (kg)	H	hydrogen
n	excess air ratio (-)	M	moisture
P	pressure (kPa)	N	nitrogen
K	percentage ratio of element in chemical composition (%)	S	sulphur
s	entropy (kJ/kg K)	steo.	stekiometric
T	temperature (K or °C)	tot.	total
ψ	specific exergy (kJ/kg-flue gas)	O	oxygen
R	universal gas constant (kJ/kg K)	0	reference point

$$H + 0.25(O_2 + 3.76\,N_2) \rightarrow 0.5H_2O + 0.94\,N_2 \qquad (2)$$

$$S + (O_2 + 3.76N_2) \rightarrow SO_2 + 3.76N_2 \qquad (3)$$
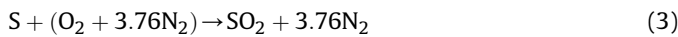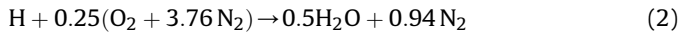
It is known that nitrogen is reacted with oxygen over about 1200 °C. In calculations, the upper limit of the flue gas temperature is assumed as 1200 °C. Combustion process is assumed as in ideal case. So, nitrogen is not considered to react with oxygen during combustion reaction. Complete combustion by using excess air can be expressed as follows:

$$C + (1+\lambda)\,(O_2 + 3.76\,N_2) \rightarrow CO_2 + (1+\lambda)\,(3.76\,N_2) + \lambda O_2 \qquad (4)$$

$$H + (1+\lambda)\,(O_2 + 3.76\,N_2) \rightarrow 0.5H_2O + (1+\lambda)\,(3.76\,N_2) \\ + (0.75+\lambda)O_2 \qquad (5)$$

$$S + (1+\lambda)\,(O_2 + 3.76N_2) \rightarrow SO_2 + (1+\lambda)\,(3.76N_2) + \lambda O_2 \qquad (6)$$
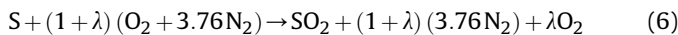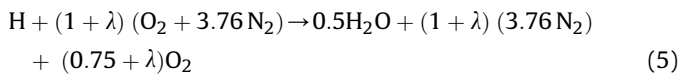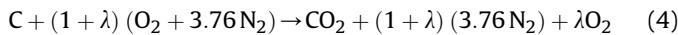
In combustion reaction, λ is the fraction of excess combustion air and n equals to $1 + \lambda$.

The mass balance equation can be expressed in the rate form as,

$$m_{in} = m_{out} \qquad (7)$$

where m is the mass flow rate, and the subscript in stands for inlet and out for outlet.

$$m_{fuel} + m_{air} = m_{flue\ gas} + m_{ash} \qquad (8)$$

$$m_{flue\ gas} = m_{fuel} + m_{air} - m_{ash} \qquad (9)$$

Required air amount can be calculated by below equation depending on excess air ratio and chemical composition of fuel.

$$m_{air} = (2.9978 \cdot K_H - 0.3747 \cdot K_O + 0.3747 \cdot K_S \\ + K_C) \cdot (11.445 \cdot n) \qquad (10)$$

Steometric air amount ($n = 1$) can be found as follows;

$$m_{air\ steo.} = (2.9978 \cdot K_H - 0.3747 \cdot K_O + 0.3747 \cdot K_S \\ + K_C) \cdot (11.445) \qquad (11)$$

Eq. (10) is obtained by employing combustion mass balance equations. Here, K denotes the percentage ratio of the element in chemical composition (in %). m_{air} means the air requirement per kg fuel (kg air/kg fuel). Flue gas amount can be found by below equation

$$m_{flue\ gas} = (2.9978 \cdot K_H - 0.3747 \cdot K_O + 0.3747 \cdot K_S \\ + K_C) \cdot (11.445 \cdot n) + \left(m_{fuel} - K_{ash}\right) \qquad (12)$$

Calculations are done for 1 kg fuel, so the equation can be expressed as follows:

$$m_{flue\ gas} = (2.9978 \cdot K_H - 0.3747 \cdot K_O + 0.3747 \cdot K_S \\ + K_C) \cdot (11.445 \cdot n) + (1 - K_{ash}) \qquad (13)$$

When $n = 1$, flue gas amount can be given by the following equation;

$$m_{tot.\ steo.} = m_{air\ steo.} + (1 - K_{ash}) \qquad (14)$$

All the calculations used here have the following characteristics: Flue gas temperature changes between 100 °C and 1200 °C.

2.2. Calculation of flue gas specific heat capacity

The specific heat values of gases found in flue gas are required to be known to obtain the average specific heat capacity (C_p) of flue gas. Taking these values from thermodynamic tables, a model is formed. The reference combustion reaction is required to generate one formulation in energy balance. Since carbon is an element found almost in all fossil fuels, the combustion reaction is considered to be a reference reaction for the model. Then, the specific heat values of all gases are defined depending on carbon dioxide. For that purpose, model coefficients are defined and expressed in detail as follows.

$$C_{p,\ flue\ gas} = \frac{C_{p,C}}{(a_C + b_N + c_H + d_S)} \cdot \frac{m_{tot.\ steo.}}{m_{flue\ gas}} + f_A \qquad (15)$$

a, b, c, d and f are the model coefficients in Eq. (15). $C_{p,\ flue\ gas}$ represents the average flue gas specific heat value. $C_{p,C}$ is the specific heat of CO_2.

2.2.1. Estimation of coefficient 'a_C'
Calculation method of a_C is given by the following equation:

$$a_C = \frac{a_m}{a_{cp}} \qquad (16)$$

where, a_{cp} can be defined as the specific heat ratio of CO_2 to CO_2. So, a_{cp} equals to 1. a_m can be indicated as the mass ratio of CO_2 to flue gas for $n = 1$.

$$a_m = \frac{m_C}{m_{tot.\ steo.}} = \frac{3.667 \cdot K_C}{m_{tot.\ steo.}} \tag{17}$$

2.2.2. Estimation of coefficient 'b_N'

Calculation method of b_N is given by the following equation:

$$b_N = \frac{b_m}{b_{cp}} \tag{18}$$

where, b_{cp} can be defined as the specific heat ratio of CO_2 to N_2 for different temperatures. Coefficient b_{cp} is estimated by using heat capacity model. b_m can be defined as the mass ratio of N_2 to total flue gas.

$$b_{cp} = 0.9094 + 1.69 \cdot 10^{-4} \cdot T - \frac{11135}{T^2} \tag{19}$$

$$b_m = \frac{m_N}{m_{tot.\ steo.}} = \frac{0.767(2.9978 \cdot K_H - 0.3747 \cdot K_O + 0.3747 \cdot K_S + K_C) \cdot (11.445) + K_N}{m_{tot.\ steo.}} \tag{20}$$

2.2.3. Estimation of coefficient 'c_H'

c_H Coefficient can be expressed as in the following equation:

$$c_H = \frac{c_m}{c_{cp}} \tag{21}$$

where, c_{cp} can be defined as the specific heat ratio of CO_2 to H_2O for different temperatures. Coefficient c_{cp} is estimated by using Heat Capacity Model. c_m can be defined as the mass ratio of H_2O to total flue gas.

$$c_{cp} = 0.5657 - 6.68 \cdot 10^{-6} \cdot T - \frac{10465}{T^2} \tag{22}$$

$$c_m = \frac{m_H}{m_{tot.\ steo.}} = \frac{8.938 \cdot K_H + K_M}{m_{tot.\ steo.}} \tag{23}$$

2.2.4. Estimation of coefficient 'd_S'

Coefficient d_S can be expressed as in the following equation:

$$d_S = \frac{d_m}{d_{cp}} \tag{24}$$

where, d_{cp} can be defined as the specific heat ratio of CO_2 to SO_2 for different temperatures. Coefficient d_{Cp} is estimated by using Vapor Pressure Model. d_m can be defined as the mass ratio of SO_2 to total flue gas.

$$d_{Cp} = e^{\left[2.679 - \frac{151.16}{T} - 0.289 \ln(T)\right]} \tag{25}$$

$$d_m = \frac{m_S}{m_{tot.\ steo.}} = \frac{2 \cdot K_S}{m_{tot.\ steo.}} \tag{26}$$

2.2.5. Calculation of coefficient 'f_A'

Coefficient f_A is calculated for access air amount. Coefficient f_A can be expressed as in the following equation

$$f_A = f_m \cdot C_{p,A} \tag{27}$$

$$C_{p,A} = 0.7124 \cdot 1.00011^T \cdot T^{0.051} \tag{28}$$

$$f_m = \frac{m_{air\ steo.} \cdot (n - 1)}{m_{flue\ gas}} \tag{29}$$

2.2.6. Calculation of C_{p,C}

$C_{p,C}$ denotes the specific heat of CO_2. Specific heat value of CO_2 is taken [18] and adopted as a new parabola by using hoerl model.

$$C_{p,C} = (0.1874) \cdot 1.000061^T \cdot T^{0.2665} \tag{30}$$

The specific heat values of some known gases were calculated for $n = 1$ and given in Fig. 1. The effect of the excess air ratio on the specific heat is demonstrated in Fig. 2 for natural gas.

2.3. Flue gas specific exergy value

The flow exergy of flue gas can be expressed in the ratio form as [19]:

$$\psi = (h - h_0) - T_0(s - s_0) \tag{31}$$

where ψ is the flow exergy, s is the specific entropy and the subscript zero indicates the properties at the dead state of P_0 and T_0. Entropy difference can be expressed in the form as

$$s - s_0 = C_p \cdot \ln\frac{T}{T_0} - R_{ave.} \cdot \ln\frac{P}{P_0} \tag{32}$$

where, R_{ave} is the average universal gas constant value of flue gas. Each gas has different gas constant. So, the average universal gas

$$R_{ave.} = \frac{K_C \cdot (0.6927) + K_N \cdot (0.2968) + K_H \cdot (4.1249) + K_S \cdot (0.2596) + K_M \cdot (0.4615) + m_{air\ steo.} \cdot (0.2201)}{m_{flue\ gas}} + \frac{(m_{air\ steo.} \cdot (n - 1) \cdot (0.287))}{m_{flue\ gas}} \tag{33}$$
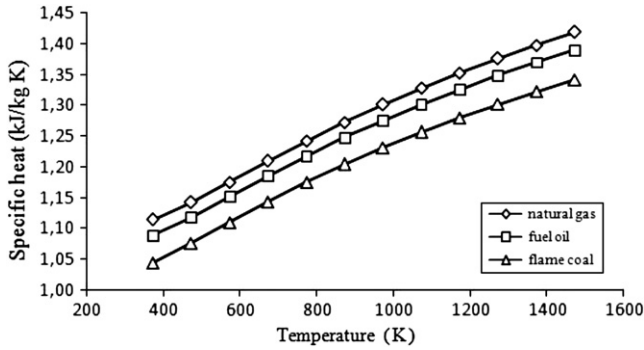
Fig. 1. Versus of the flue gas specific heat capacity values for different fuels ($n = 1$).

Table 1
Elemental analysis of lignite coal.

Elemental analysis (%)						
C	H	O	N	S	Moisture	Ash
51.12	3.89	14.65	0.61	1.87	14.36	13.5

constants of combustion products are calculated and given in the Eq. (31) below.

Employing the new approach, the universal gas constants of flue gas were calculated for some known fuels and given in Fig. 3. As it can be seen from Fig. 3, when excess air ratio increase, the average flue gas universal gas constant tends to approach gas constant of air (0.287 kJ/kg K).

$$\psi = C_{p,\text{flue gas}} \cdot (T - T_0) - T_0 \left(C_{p,\text{flue gas}} \cdot \ln \frac{T}{T_0} - R_{\text{ave.}} \cdot \ln \frac{P}{P_0} \right) \tag{34}$$

$$\psi = C_{p,\text{flue gas}} \cdot (T - T_0) - T_0 \cdot C_{p,\text{flue gas}} \left(\ln \frac{T}{T_0} - \frac{R_{\text{ave.}}}{C_{p,\text{flue gas}}} \cdot \ln \frac{P}{P_0} \right) \tag{35}$$

$$\psi = C_{p,\text{flue gas}} \cdot \left[(T - T_0) - T_0 \left(\ln \frac{T}{T_0} - \frac{R_{\text{ave.}}}{C_{p,\text{flue gas}}} \cdot \ln \frac{P}{P_0} \right) \right] \tag{36}$$

When $P \cong P_0$, general exergy flow equation can be written as;

$$\psi = C_{p,\text{flue gas}} \cdot \left[(T - T_0) - T_0 \left(\ln \frac{T}{T_0} \right) \right] \tag{37}$$

3. An application of the new approach for lignite coal

In this chapter a sample analysis for 1 kg of lignite coal was done in order for the formulas given in the calculation section to be understood well. The chemical composition of lignite is given in Table 1 and it is burned without excess air. Flue gas temperature is accepted as 1000 K for calculation.
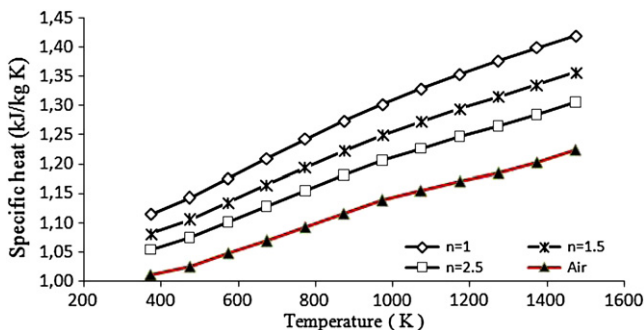
$K_{\text{H}} = 0.0389, \ K_{\text{O}} = 0.1465, \ K_{\text{N}} = 0.0061,$
$K_{\text{M}} = 0.1436, \ K_{\text{S}} = 0.0187, \ K_{\text{C}} = 0.5112$

Required air amount is found by using Eq. (10)

$$m_{\text{A}} = (2.9978 \cdot K_{\text{H}} - 0.3747 \cdot K_{\text{O}} + 0.3747 \cdot K_{\text{S}} + K_{\text{C}}) \cdot (11.445 \cdot n)$$

$$m_{\text{A}} = (0.5799) \cdot (11.445) = 6.63 \text{ kg}$$

Flue gas amount is found by using Eq. (11)

$$m_{\text{flue gas}} = (2.9978 \cdot K_{\text{H}} - 0.3747 \cdot K_{\text{O}} + 0.3747 \cdot K_{\text{S}} + K_{\text{C}}) \cdot (11.445 \cdot n) + (1 - K_{\text{ash}})$$

$$m_{\text{flue gas}} = 7.4864 \text{ kg/kg fuel}$$

Calculated flue gas amount obtained from the chemical reaction is given below:

$$m_{\text{Real flue gas}} = 7.494 \text{ kg}$$

Error rate for mass can be found by the following equation.

$$\text{Error rate} = \frac{7.494 - 7.4864}{7.494} = 0.001 = 0.1\%$$

Average C_p value of flue gas at 1000 K is found by using Eq. (15). Also, changes of error rate for flue gas specific heat are calculated and given in Fig. 4.

$$C_{p,\text{flue gas}} = \frac{C_{p,\text{C}}}{(a_{\text{C}} + b_{\text{N}} + c_{\text{H}} + d_{\text{S}})} \cdot \frac{m_{\text{tot. steo.}}}{m_{\text{flue gas}}} + f_{\text{A}}$$

$$C_{p,\text{flue gas}} = \frac{1.255}{(0.2498 + 0.6366 + 0.1196 + 0.0029)} \cdot 1 + 0$$

$$C_{p,\text{flue gas}} = 1.2667 \text{ kJ/kg K}$$

Flue gas specific exergy values of lignite coal are calculated for 30 °C reference temperature and given in Fig. 5.
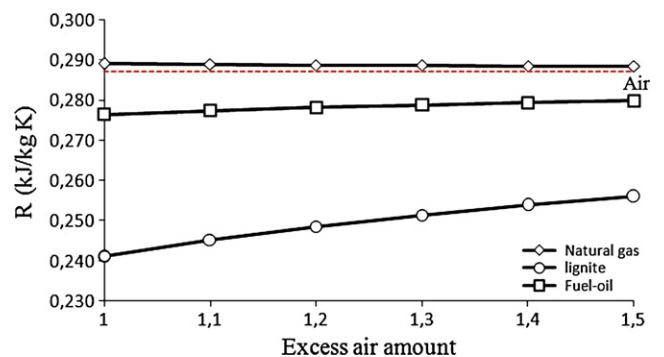

Fig. 2. Versus of specific heat capacity of flue gas for natural gas at different excess air ratio.

Fig. 3. Change of average universal gas constant of flue gas for different excess air ratio and well-known fuels.
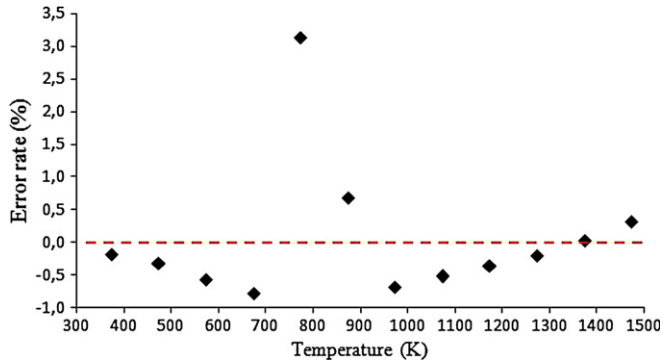
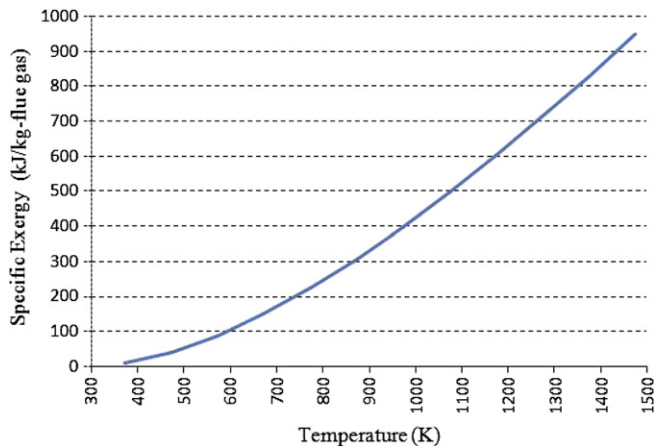**Fig. 4.** Versus of the error rate for lignite coal.

Fig. 5. Versus of the flue gas specific exergy values for lignite coal ($n = 1$).

$$\psi = C_{p,\text{flue gas}} \cdot \left[(T - T_0) - T_0 \left(\ln \frac{T}{T_0} \right) \right]$$

$$\psi = 1.2667 \cdot \left[(1000 - 303) - 303 \left(\ln \frac{1000}{303} \right) \right]$$

$$\psi = 424.6 \text{ kJ/kg} - \text{flue gas}$$

4. Conclusion

In this study, a new approach is proposed to calculate the flue gas specific heat and specific exergy value by entering the chemical composition, excess air ratio and flue gas temperature. The present approach is applicable for all carbon-based fuels, especially biomass, fossil fuels and fuel mixtures for co-combustion. Also, new formulation is given for average universal gas constant of combustion products. The researchers, designers and engineers working in the area of combustion or boiler system design such as heat exchanger, economizer and air-heater design can utilize this model for the accurate estimation of flue gas exergy value. Model error rate is calculated for lignite combustion products. It was noted that error rate reach as high as 3%.

Concluding remarks;

- When excess air ratio increase, both average flue gas universal gas constant and average specific heat of flue gas tend to approach air values.
- Specific heat capacity of flue gas for each different composition has a similar trend but different values.

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