

# ALGORITHMS APPLIED IN FLAME TEMPERATURE CALCULATION

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**ABSTRACT:** This paper presents data on hydrocarbon combustion stoichiometry and algorithms for determining flame temperature. If that does not take into account the dissociative reaction products (CO<sub>2</sub>, H<sub>2</sub>O and N<sub>2</sub>) algorithm allows the calculation of the flame temperature of the heat balance equation. It analyzes the general case of dissociative-products CO<sub>2</sub> and H<sub>2</sub>O. In this case we apply a different algorithm that solve a system of nonlinear equations with six unknowns  $\nu_{CO_2d}$ ,  $\nu_{COd}$ ,  $\nu_{H_2Od}$ ,  $\nu_{H_2d}$ ,  $\nu_{OHd}$ ,  $\nu_{O_2d}$  then apply the first algorithm to determine the flame temperature. When burning natural gas with the initial conditions  $t_0 = 15$  C and pressure of the atmosphere resulting  $t_f = 2049.246$  C under the same conditions, with consideration of dissociation,  $t_f = 2049.822$  C. Algorithms do not use iterative solution of the equation of thermal balance.

**KEYWORDS:** Stoichiometric combustion, Thermodynamics

## 1. INTRODUCTION

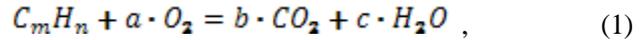
Efficient combustion of gaseous fuels is a major issue which requires attention on burning gaseous fuels in industrial installations in order to achieve a fuel savings as high. How to carry out the combustion process, leading to the achievement of quality products in the various processes.

In the majority of plants which use combustion of fuel gas is used diffusion (diffusion flame), which is characterized in that the mixing between fuel gas and combustion air is carried out just in the area of combustion, two jets (gaseous fuel and air) are introduced separately into the combustion chamber.

In order to obtain diffusion flames, with features allowing various processes to achieve optimal conditions, it is necessary to know the physical, chemical and geometrical characteristics influencing the flame. Knowledge of these factors and how they influence may lead to the development of fire with well-defined characteristics in the different stages of these processes.

Air needed for combustion, as the composition of the combustion products are determined by the equation expressing global fuel oxidation reactions, respecting the principle of conservation of mass for each of the elements of reactants.

If the fuel composition is a hydrocarbon  $C_mH_n$  generated global full oxidation reaction has the form



where stoichiometric ratios (1, a, b, c) are expressed in moles.

Conservation of mass of carbon is expressed by the condition

$$b = m,$$

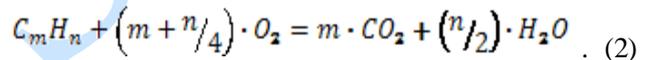
and hydrogen in the condition

$$c = n/2.$$

Conservation of mass requires oxygen provided

$$a = m + n/4.$$

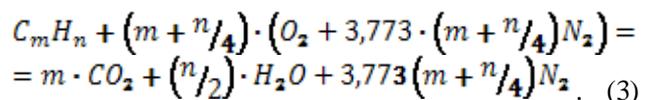
Equation (1) takes the form



Dry atmospheric air contains 20.95% (volume) oxygen, 78.09% nitrogen, 0.93% argon, the other components being considered negligible proportions. The usual calculations that follow define the thermodynamic properties of the reactants and products are neglected and the presence of argon, considering that air consists of 21% (vol.) and oxygen and 79% nitrogen, expressed in moles.

For each mole of oxygen is considered  $(1 - 0.2095) / 0.2095 = 3.773$  mole of nitrogen.

The normal calculation is considered that the nitrogen does not participate in the combustion reaction. Therefore, the equation for the complete combustion in the ambient air, hydrocarbon  $C_mH_n$  has the form



## 2. FLAME TEMPERATURE CALCULATION

A simple steady-state thermal energy balance can be constructed around a constant-pressure combustion system.

The figure 1 presents the energy balance of the combustion system.

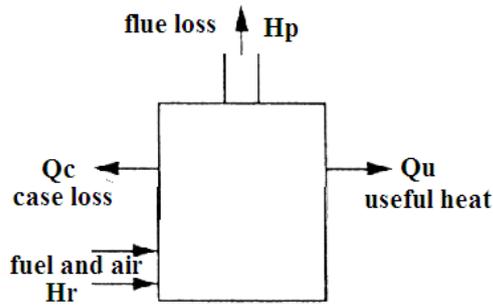


Fig. 1 Combustion system diagram

### 3. ADIABATIC FLAME TEMPERATURE

The energy balance about the system can be written as:

$$HR + CVFuel = HP + Qc + Qu \quad (4)$$

where

CVFuel – calorific value,

HR- the sensible heat in the air and fuel (is very small and often neglected),

HP - enthalpy of reaction products.

Table 1. Lower and Higher Heating Values of Gas Fuels

Fuels (Gaseous Fuels 0 °C and 1 atm)	Lower Heating Values LHV - [Mj/kg]	Higher Heating Values HHV - [Mj/kg]
Natural gas	47.141	52.225
Hydrogen	120.21	142118
Still gas	46.898	50.951

The case loss from the outside of the plant,  $Q_c$ , is also generally small compared to the other energy fluxes and is similarly often considered negligible.

It is assumed that combustion takes place under adiabatic conditions, i.e. no heat transfer is permitted across the boundary of the system.

The implication of this is that

$$Q_c = 0,$$

and

$$Q_u = 0.$$

Hence equation (4) simplifies down to

$$HR + CVFuel = HP \quad (5)$$

### 4. MOLAR ISOBARIC HEAT

It adopts the form isobaric molar heat:

$$C_p(T) = a_1 + a_2 \cdot T + a_3 \cdot T^2 + a_4 \cdot T^3 \quad (6)$$

For the reactants and products the isobaric molar heat depending on temperature, where the measure

unit is  $\left[ \frac{kJ}{kmol \cdot K} \right]$ , are:

- for CH<sub>4</sub>

$$C_{pCH4}(T) = 16,716 + 0,071T - 1,941 \cdot 10^{-5}T^2 - 1,768 \cdot 10^{-9}T^3,$$

- for O<sub>2</sub>

$$C_{pO2}(T) = 33,719 + 6,968 \cdot 10^{-4}T + 8,397 \cdot 10^{-7}T^2 - 1,269 \cdot 10^{-10}T^3,$$

- for CO<sub>2</sub>

$$C_{pCO2}(T) = 30,857 + 0,03T - 9,189 \cdot 10^{-6}T^2 - 9,072 \cdot 10^{-10}T^3,$$

- for H<sub>2</sub>O

$$C_{pH2O}(T) = 28,14 + 0,016T - 3,006 \cdot 10^{-6}T^2 + 1,899 \cdot 10^{-10}T^3,$$

- for N<sub>2</sub>

$$C_{pN2}(T) = 26,529 + 7,979 \cdot 10^{-3}T - 2,002 \cdot 10^{-6}T^2 + 1,724 \cdot 10^{-10}T^3,$$

- for CO

$$C_{pCO}(T) = 26,535 + 0,009 \cdot T,$$

- for OH

$$C_{pOH}(T) = 28,386 + 0,003 \cdot T,$$

- for H<sub>2</sub>

$$C_{pH2}(T) = 27,581 + 0,003 \cdot T.$$

### 5. CALCULATION ALGORITHM

A straight forward method for the calculation of adiabatic flame temperature is to execute the following steps:

(1) It evaluates both sides of the equation

$$HR + CVFuel = HP;$$

where HR is the enthalpy sensitive, CV is calorific value and HP is the enthalpy of reaction products,

$$HR = HRO_2 + HRN_2, \quad CVFuel = CVCH_4,$$

$$HP(T_f) = HPCO_2(T_f) + HPH_2O(T_f) + HPN_2(T_f).$$

(2) solve the equation with unknown Tf  
 $HP(Tf) - (HR + CVFuel) = 0$  (7)  
 using Mathcad root function.

**6. CASE STUDY. ANALYSIS WITHOUT CONSIDERATION DISSOCIATION REACTION PRODUCTS**

Find the adiabatic flame temperature for a stoichiometric methane/air flame if the initial temperature of the fuel and air is 5, 10, 15, 20 and 25 °C.  
 Take the net calorific value of methane as

$$CVCH4 = 16 \cdot 50 \cdot 14 \cdot 10^6 \left[ \frac{J}{kmol} \right]. \quad (8)$$

The initial temperature of the fuel and air

$$i = 1..5, T1(i) = 273.16 + 5 \cdot i, t1(i) = 5 \cdot i$$

**Table 2. Initial temperatures of fuel and air**

i	t1(i)	T1(i)
1	5	278.16
2	10	283.16
3	15	288.16
4	20	293.16
5	25	298.16

Standard temperature  $ts = 25^\circ C$ ,  
 $Ts = 273.16 + ts$ ,  $Ts = 298.16 [K]$ .  
 The first step is to evaluate, for 1 kmol of methane:

$$\begin{aligned} vCH4 &= 1, vRO2 = 2, vRN2 = 7.524, \\ HCH4(i) &= \int_{Ts}^{T1(i)} vCH4 \cdot CpCH4(T) \cdot dT, \\ HRO2(i) &= \int_{Ts}^{T1(i)} vRO2 \cdot CpO2(T) \cdot dT, \\ HRN2(i) &= \int_{Ts}^{T1(i)} vRN2 \cdot CpN2(T) \cdot dT, \\ HR(i) &= HCH4(i) + HRO2(i) + HRN2(i), \\ vPCO2 &= 1, vPH2O = 2, vRN2 = 7.524, \\ HPCO2(Tf) &= \int_{Ts}^{Tf} vPCO2 \cdot CpCO2(T) \cdot dT, \\ HPH2O(Tf) &= \int_{Ts}^{Tf} vPH2O \cdot CpH2O(T) \cdot dT, \\ HPN2(Tf) &= \int_{Ts}^{Tf} vPN2 \cdot CpN2(T) \cdot dT, \\ HP(Tf) &= HPCO2(Tf) + HPH2O(Tf) + HPN2(Tf). \end{aligned} \quad (9)$$

Solving equation (7)

$$\begin{aligned} i &= 1..5 \\ S(Tf, i) &= HP(Tf) - (CVCH4 + HR(i)) \\ Tf &= 2000 \\ Tf(i) &= \text{root}(S(Tf, i), Tf) \\ tf(i) &= Tf(i) - 273.16 \end{aligned} \quad (10)$$

The calculated CH4 flame temperature is presented in table 3, depending on initial fuel and air temperature.

**Table 3. Flame temperature**

i	Initial temperature CH4 / air		CH4 Flame temperature calculated	
	T1(i) [K]	t1(i) [°C]	TfCH4(i) [K]	tfCH4(i) [°C]
1	278.16	5	2315.152	2041.992
2	283.16	10	2318.776	2045.616
3	288.16	15	2322.406	2049.246
4	293.16	20	2326.042	2052.882
5	298.16	25	2329.683	2056.523

**7. DISSOCIATION REACTION PRODUCTS**

The dissociation equilibrium constant Cp for CO2, H2O and OH reaction components is presented in table 4.

**Table 4. Cp for CO2, H2O and OH**

Td [K]	KpCO2(Td)	KpH2O(Td)	KpOH(Td)
2500	3944.194	9.244	0.942
2750	1970.416	5.951	1.003
3000	984.368	3.831	1.067
3250	598.843	2.794	1.115

**8. ALGORITHM FOR DETERMINING THE DISSOCIATION REACTION PRODUCT WITH CONSIDERATION OF CO2 AND H2O**

It adopts

$$k = 0..3, Td(k) = 2500 + 250 \cdot k, p = 10^5,$$

Estimated values for the unknown

$$\begin{aligned} vCO2d &= 0.9, vCOd = 0.1, vH2Od = 1, \\ vH2d &= 0.1, vOHd = 0.1, vO2d = 0.1 \end{aligned}$$

Given

$$\begin{aligned} vCO2d + vCOd &= 1 \\ vH2Od + vH2d + \frac{1}{2}vOHd &= 2 \end{aligned}$$

$$vCO2d + \frac{1}{2}vCOd + \frac{1}{2}vH2Od + vO2d + \frac{1}{2}vOHd = 2$$

$$\frac{vCO2d}{vCO2d \cdot vO2d^{\frac{1}{2}}} \cdot \left( \frac{p}{vCO2d + vCOd + vO2d} \right)^{-\frac{1}{2}} = KpCO2(T(i))$$

$$\frac{vH2Od}{vH2d \cdot vO2d^{\frac{1}{2}}} \cdot \left( \frac{p}{vH2Od + vH2d + vO2d} \right)^{-\frac{1}{2}} = KpH2O(T(i))$$

$$\frac{vOHd}{vH2d \cdot vO2d^{\frac{1}{2}}} = KpOH(T(i))$$

$$Sol(i) = Find(vCO2d, vCOd, vH2Od, vH2d, vOHd, vO2d)$$

$$vCO2d(k) = Sol(k)_1, vCOd(k) = Sol(k)_2,$$

$$vH2Od(k) = Sol(k)_3,$$

$$vH2d(k) = Sol(k)_4, vOHd(k) = Sol(k)_5,$$

$$vO2d(k) = Sol(k)_6,$$

Table 5.

k	Td(k) [K]	vCO2d(k)	vCOd(k)	vH2Od(k)
1	2500	0.999989	0.000011	1.982456
2	2750	0.99998	0.00002	1.976076
3	3000	0.999965	0.000035	1.967379
4	3250	0.999948	0.000052	1.959285

Table 6.

k	Td(k) [K]	vH2d(k)	vOHd(k)	vO2d(k)
1	2500	0.013682	0.007724	0.004916
2	2750	0.018441	0.010966	0.006489
3	3000	0.024844	0.015554	0.008551
4	3250	0.030741	0.019948	0.010409

## 9. FLAME TEMPERATURE CALCULATION BASED ON PARAMETERS i AND k

Algorithm is applied to paragraph 7 of reaction products calculated by considering the dissociation

$$HPCO2d(Tf, k) = \int_{T_s}^{T_f} vPCO2d(k) \cdot CpCO2(T) \cdot dT$$

$$HPH2Od(Tf, k) = \int_{T_s}^{T_f} vPH2Od(k) \cdot CpH2O(T) \cdot dT$$

$$HPN2d(Tf, k) = \int_{T_s}^{T_f} vPN2d(k) \cdot CpN2(T) \cdot dT$$

$$HPH2d(Tf, k) = \int_{T_s}^{T_f} vPH2d(k) \cdot CpH2(T) \cdot dT$$

$$HPOHd(Tf, k) = \int_{T_s}^{T_f} vPOHd(k) \cdot CpOH(T) \cdot dT$$

$$HPO2d(Tf, k) = \int_{T_s}^{T_f} vPO2d(k) \cdot CpO2(T) \cdot dT$$

$$HR(i) = HCH4(i) + HRO2(i) + HRN2(i),$$

$$HP(Tf, k) = HPCO2d(Tf, k) + HPH2Od(Tf, k) + HPN2d(Tf, k) + HPH2d(Tf, k) + HPOHd(Tf, k) + HPO2d(Tf, k),$$

(11)

$$HP(Tf, k) - (HR(i) + CVFuel) = 0$$

(12)

To solve the equation (11) with unknown Tf, and i and k parameters using Mathcad root function

$$i = 1..5, k = 0..3$$

$$Sd(Tf, i, k) = HP(Tf, k) - (CVCH4 + HR(i))$$

$$Tf = 2200$$

$$Tfd(i, k) = root(Sd(Tf, i, k), Tf)$$

$$tfd(i, k) = Tfd(i, k) - 273.16$$

(13)

Numerical values obtained are presented in table 7 and table 8.

Table 7.

i	Tfd(I,0) [K]	Tfd(I,1) [K]	Tfd(I,2) [K]	Tfd(I,3) [K]
1	2314.728	2314.576	2314.371	2314.18
2	2318.352	2318.2	2317.371	2317.804
3	2321.982	2321.83	2321.624	2321.434
4	2325.617	2325.465	2325.26	2325.069
5	2329.258	2329.107	2328.901	2328.71

Table 8.

i	tfd(I,0) [°C]	tfd(I,1) [°C]	tfd(I,2) [°C]	tfd(I,3) [°C]
1	2041.568	2041.416	2041.211	2041.02
2	2048.192	2045.04	2044.835	2044.644
3	2049.822	2048.67	2048.464	2048.274
4	2052.457	2052.305	2052.1	2051.909
5	2056.098	2055.947	2055.741	2055.55

## CONCLUSIONS

The presented algorithm for reaction products determination, with CO2 and H2O dissociation can be used also for H2, O2 and N2 dissociation. In this case there are nine unknowns.

In the study of combustion, there are two types of adiabatic flame temperature depending on how the process is completed, constant volume and constant pressure, describing the temperature the combustion products theoretically reach if no energy is lost to the outside environment.

The constant volume adiabatic flame temperature is the temperature that results from a complete combustion process that occurs without any work, heat transfer or changes in kinetic or potential energy. The constant pressure adiabatic flame temperature is the temperature that results from a complete combustion process that occurs without any heat transfer or changes in kinetic or potential energy. Its temperature is lower than the constant volume process because some of the energy is utilized to change the volume of the system (i.e., generate work).

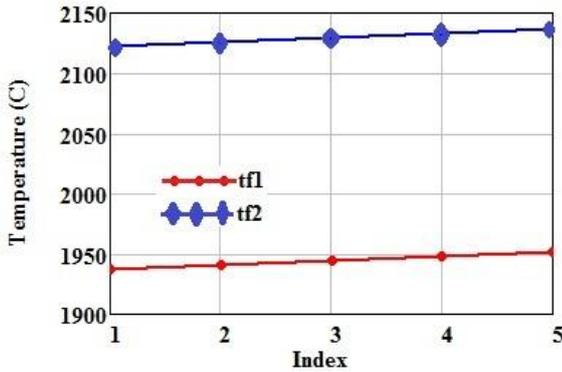


Fig. 2 Variation of flame temperature calculated according to the initial temperature CH<sub>4</sub> / air

Table 9. Higher (HHV) and Lower (LHV) Heating values of some common fuels [Lew51]

Fuel	HHV $\left[\frac{MJ}{kg}\right]$	HHV $\left[\frac{kJ}{mol}\right]$	LHV $\left[\frac{MJ}{kg}\right]$
Hydrogen	141.80	286	119.96
Methane	55.50	889	50.00
Ethane	51.90	1,560	47.80
Propane	50.35	2,220	46.35
Butane	49.50	2,877	45.75
Pentane	--	--	45.35
Gasoline	47.30	--	--

The higher heating value takes into account the latent heat of vaporization of water in the combustion products, and is useful in calculating heating values for fuels where condensation of the reaction products is practical (e.g., in a gas-fired boiler used for space heat).

If the gross calorific value is used, then  $H_R$  should contain a latent heat term equal to the mass of water produced per kilogram of fuel multiplied by the latent heat of evaporation of water at 25 °C ( $h_{fg}$ ).

If the net calorific value is used, then the flue gas enthalpy will consist of sensible heat terms only.

We are concerned with predicting the temperature reached within the flame, hence the net calorific value/sensible heat terms system is the more appropriate.

Table 10. Flame temperatures for some common fuels

Fuel	Adiabatic flame temperature [°C]
Natural gas	2070
Kerosine	2093
Light fuel oil	2104
Medium fuel oil	2101
Heavy fuel oil	2102
Bituminous Coal	2172
Anthracite	2180

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