

# Determination of Adiabatic Flame temperature of a Conventional Cupola Furnace Effects of Excess Air on the Flue Gases Specific Heat

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## Abstract

A thermal analysis was carried out on a 6.5m tall and 0.65m diameter conventional cupola furnace at the Nigeria Railway Corporation, Enugu. A combustion and thermal analysis of the fuel (coke) used for its operation has been carried out and the adiabatic combustion temperature of the fuel has been determined to be 2,175.93K. The stoichiometric and actual air-fuel ratio of the furnace were found to be 10.97 and 12.08 respectively. The percentage excess air was varied from 0.05 (5%) to 1.2 (120%) to determine their effects on the Cp of the gases considering both wet and dry basis analysis. The percentage excess air was varied from 0.05 (5%) to 1.2 (120%) to determine their effects on the Cp of the gases considering both wet and dry basis analysis. The CO<sub>2</sub> and N<sub>2</sub> shown decreasing and increasing trend respectively as the percentage excess air increase. Both coincide at 0.43 (43%) excess air. The behavior of oxygen and water vapour from the combustion also shows the same trend but had their intercept at 0.39 (39%) excess air. The percentage of flue gases difference for wet and dry case were also investigated against the percentage excess air. The N<sub>2</sub> and CO<sub>2</sub> curves intercepted at the point of 0.44 (44%). The permissible maximum of 45% (with range of 30% - 45%) excess air is required for the real balanced combustion in the furnace to give the system specified output without the dissociation of the gases and as well as the system's metallurgical consideration.

**Keywords:** *cupola furnace, thermal analysis, combustion, excess air, adiabatic temperature*

## Introduction

Metal production and reproduction is a major aspect of the manufacturing industry as metals are used extensively in manufacturing due to their strength and other properties. Production of these metals or alloys in the specific shapes and sizes require certain processes like casting, machining, welding and other mechanical work, with casting being the primary process.

The cupola furnace is mostly used for heating metals with very high melting temperature and for heating over a long period of time due to its design. It is commonly used by metal manufacturing and recycling companies.

Cupola furnace is one of the oldest methods of melting steel scrap, cast iron scrap and ferroalloys to produce cast iron [1]. Other melting methods like electric induction melting have led to the decline of

the use of the cupola, but the cupola has remained dominant because of its many attractive characteristics [2]. Due to the wide use of the cupola furnace, designers and researchers have found it necessary to work towards the improvement of the design of the cupola furnace for better production, lower cost, and lower emissions.

The cupola furnace is a type of furnace used widely in foundries for melting of high melting point metals to produce their cast forms. The name cupola furnace was derived from the resemblance of the furnace to the cupola commonly found on top of dwelling houses [3]. It uses fuels with high heating values like coke, charcoal, natural gas for heating. As it is evident that the cupola furnace is subjected to temperature in excess of 1300K, it can be termed a trimmed down version of the well-known blast furnace [4].

The cupola furnace is a cylindrical shaped steel furnace lined with refractories or water-cooled surfaces depending on the type of fuel used. The name coke cupola resulted from the wide use of coke as the solid fuel in cupolas [5]. Gas cupolas heat faster and more efficiently and are used more in melting of steel, but has great setback in the cost and availability of gas supply, and requires high precaution during operation [6].

The solid fuel cupolas could use fuels like coal, coke or charcoal and different foundries choose either of them for various reasons. The choice of fuels depends on its needed properties like the carbon content (chemical), calorific value (thermal), economic value, etc. Coke widely used as solid fuel in cupolas is a hard carbon material produced by destructive distillation of coal (mostly bituminous coal) in an airless oven at very high temperature (usually 1000 – 1100°C) [7].

### **Cupola furnace design**

The design and fuel used for cupola operation is subject to the material to be melted, as they melt different types of metals including steel. Cast iron mostly melted in cupolas due to its wide use in production has a specific heat of 0.42 to 0.73kJ/kg.K, latent heat of fusion of 96.3kJ/kg and a melting temperature of 1573K [8,9]. The metal composition needed for particular production/casting makes the selection of charge materials (fuel, metal and flux) very important in the cupola operation. Limestone charged with the metal scrap in cupolas undergoes thermal decomposition to form lime which acts as flux, ridding impurities off the metal to form slag. Limestone has a specific heat of 0.91kJ/kg.K, latent heat of fusion of 57.35kJ/kg and a melting temperature of 1098K [8,10].

There are three basic zones in the cupola furnace – the stack zone, the melt zone (combustion zone), and the well zone [11], while other researchers identify zones like the reducing and preheating zone in the stack and combustion zone [12]. The design of cupolas allows the charge materials to start heating up at the stack zone before entering the melt zone using heat from the combustion gases moving up the column, hence the term preheating zone [3].



*Fig. 1* Pictorial view of a conventional Cupola Furnace, source [13].

### **Cupola Furnace Improvements**

Over the years, there have been much research work and improvement on the cupola furnace which covers areas like design, operation and fuel with the aim of better production and reduced cost. Some of these improvements are discussed further.

#### **i. Divided Blast Cupola**

This is simply a design that splits the air supply to the cupola into two levels, one below the coke bed and the other at some distance above the coke level. The divided blast reduces coke consumption by 20 – 32%, increases melting rate of metal by 11 – 23%, increases metal tapping temperature by 40 – 50°C and increases carbon pickup by approximately 0.06% [14]. Air needed for combustion is normally fed through the tuyeres below the coke bed. This air fed speeds up the combustion of coke alone leaving the metal to melt slowly, but when air is divided and supplied at the metal level, it quickens the combustion and melting of metal, thereby reducing the consumption of coke.

#### **ii. Preheated Blast and Oxygen Enrichment**

The preheated blast involves the use of hot air for combustion instead of the conventional cold air blown directly from the blower. This is achieved by attaching either a heater to the air-box which heats the air from the blower before getting into the furnace through the tuyeres, or a heat recuperating system (heat exchanger) which collects heat from the cupola emitted gases and sends it back to the cupola with the blown air as hot air [11].

Oxygen enrichment involves the introduction of oxygen from an attached source to the combustion chamber. The efficiency of the cupola in some works has been increased by 10% and above with the use of oxygen enrichment [15, 16].

#### **iii. Air Pollution (Emission) Control:**

Cupolas have been associated with high emission due to the chemical reactions taking place in its combustion chamber. This has raised alarm in many countries and has caused foundries to move to the use of induction furnaces. The control of emissions in cupolas has led to improvements in the cupola design. The emission control devices include baghouses and the wet scrubbers like the Teri's

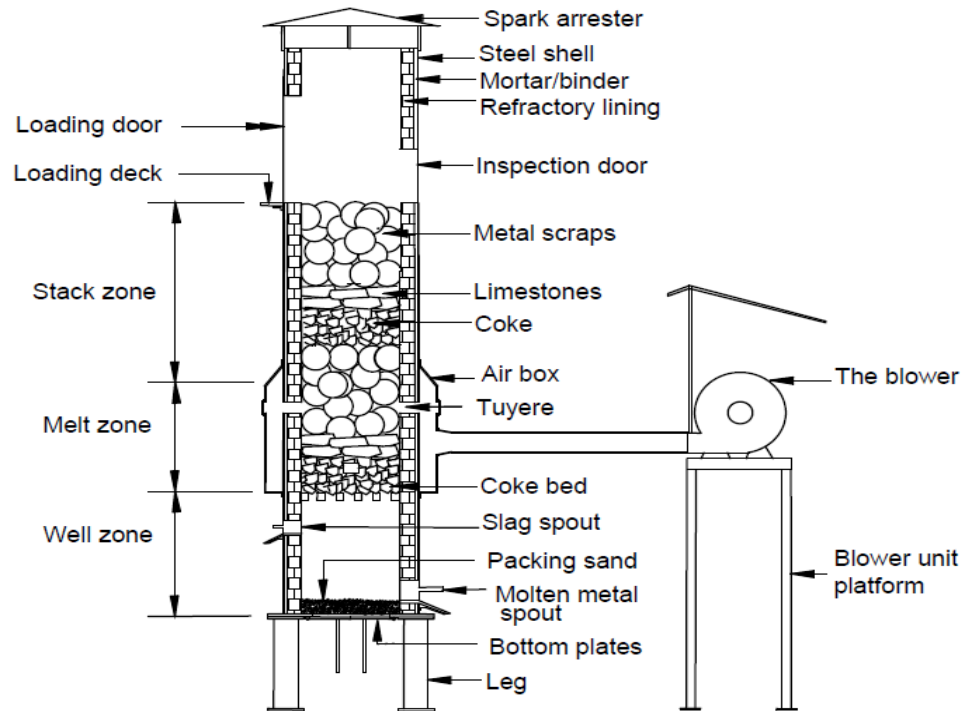
Venturi Scrubber system [13]. These devices trap harmful gases from the cupola and filter them before release to the atmosphere.

### System brief description

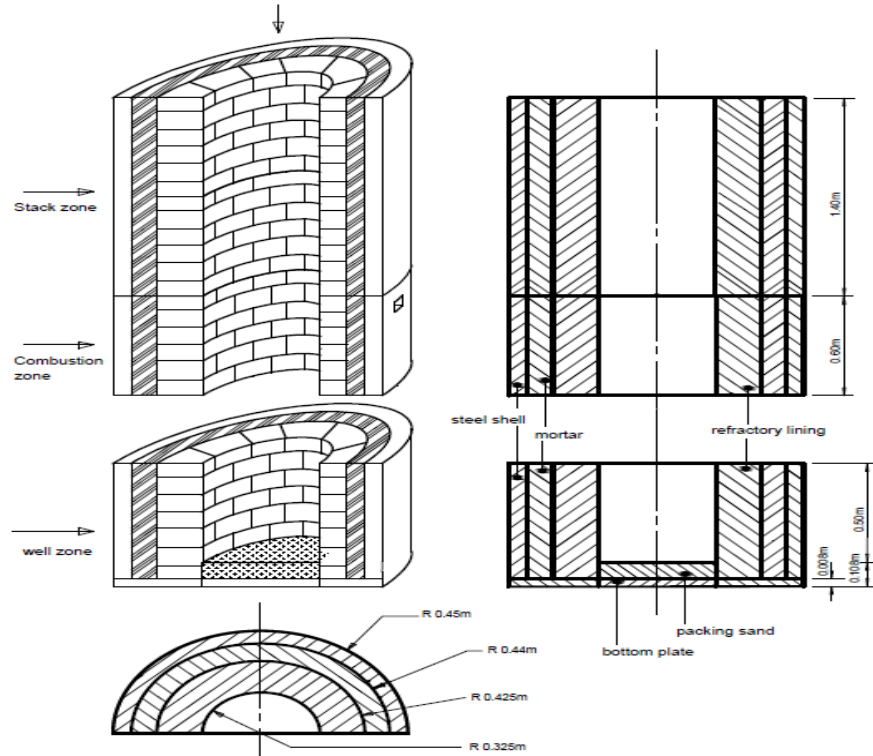
A conventional cupola furnace at the Nigeria Railway Corporation, Enugu was used for this study. A description of this furnace is discussed here as the first step in a thermodynamic analysis which must be the definition of the entity (system) that is being subjected to analysis.

The cupola is 6.5m in height, has an internal diameter of 0.65m with thickness of 12.5cm. It consists mainly of the shell (casing), the refractory lining, and the blower unit and uses coke as fuel for its operation, melts mostly cast iron scraps used in the production of grey cast iron train parts (e.g. brake pads) and other railway accessories. Schematic diagram of the furnace is shown in Figure 2 and dimensions of the furnace's zones are presented in the sectional views in Figure 3.

The cupola operates in batches as the charge materials are introduced and tapped periodically and each batch takes about an hour. The cupola operation uses about 45kg of coke, 120kg of limestone and 780kg of metal per batch. The main body of the furnace was made from rolling a 0.01m high carbon steel into a cylindrical shape with external diameter of 0.9m. Joining methods like welding and the use of bolts and nuts were employed to fabricate the cupola shell [15].



*Fig. 2 Schematic diagram of a conventional cupola furnace*



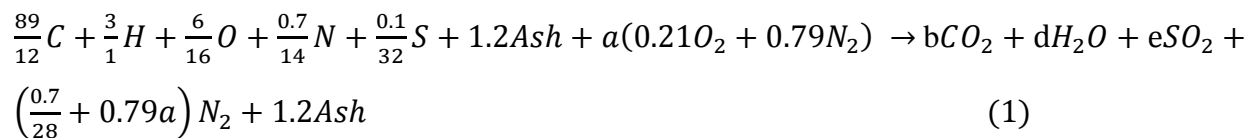
**Fig. 3** Sectional views of the zones of the furnace

**Table 1** Data for ultimate analysis of coke used

S/No.	Components of fuel	Percentage by mass %
1	Carbon, C	89
2	Hydrogen, H	3
3	Oxygen, O	6
4	Nitrogen, N	0.7
5	Sulphur, S	0.1
6	Ash and other volatile matter	1.2

### 3.3.1 Combustion Stoichiometry

The stoichiometric equation can be written as:



Determining the number of moles, a, b, d, e by material balance;

Carbon balance:  $\frac{89}{12} = b; \Rightarrow b = 7.42$

Hydrogen balance:  $2d = 3; \Rightarrow d = 1.5$

Sulphur balance:  $\frac{0.1}{32} = e = 0.003125$

Oxygen balance:  $\frac{6}{16} + 0.42a = 2b + d + 2e$

$$0.375 + 0.42a = 14.84 + 1.5 + 0.0062$$

$$a = 38.03$$

The amount of air required to burn 1kg of fuel is;

$$a \frac{(0.21 * 32 + 0.79 * 28)}{100} = 0.2884a \quad (2)$$

Therefore, the stoichiometric air/fuel ratio is;

$$AFR_{stoic} = 0.2884 * 38.03 = 10.97$$

The actual air/fuel ratio,  $R_{act}$  is given by:

$$AFR_{act} = \frac{\dot{m}_{air}}{\dot{m}_f} \quad (3)$$

$\dot{m}_{air}$  = mass flow rate of air

$\dot{m}_f$  = mass flow rate of fuel

The mass flow rate of air is obtained from the volume flow rate of the blower which is rated  $0.1275m^3/s$ .

Mass flow rate,  $\dot{m}$  = volume flow rate ( $\dot{v}$ ) \* density of air ( $\rho$ ) at 1atm,  $25^\circ C$ ;

$$\dot{m} \left( \frac{kg}{s} \right) = \dot{v} \left( \frac{m^3}{s} \right) * \rho \left( \frac{kg}{m^3} \right) \quad (4)$$

$$\dot{m}_{air} = 0.1275 * 1.184 = 0.15096kg/s$$

The mass flow rate of the fuel will amount to 0.0125kg/s based on 45kg of coke charged every 1 hour in the cupola furnace.

The actual air/fuel ratio becomes;

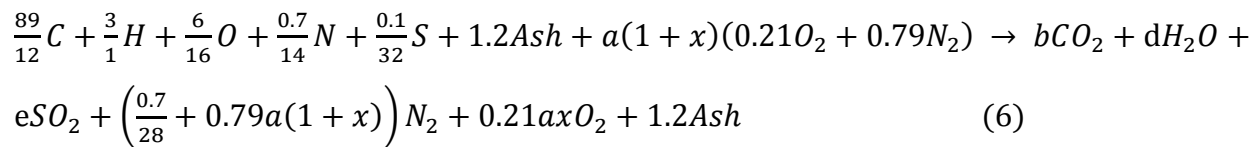
$$AFR_{act} = \frac{0.15096}{0.0125} = 12.08$$

The excess air (EA) in the combustion is given by

$$EA = \frac{AFR_{act} - AFR_{stoic}}{AFR_{stoic}} \quad (5)$$

$$\Rightarrow \frac{12.08 - 10.97}{10.97} = 0.10 \Rightarrow (10\% \text{ excess air})$$

The combustion equation with excess air can be written as:



The masses and number of moles of the reactants and the products are therefore obtained and shown in Tables 3.5 and 3.6.

**Table 2 Analysis of reactants for  $x$  – fraction of excess air**

Reactants	Atomic mass	Amt of sub./100Kg of fu	Mass per 100Kg of fu	Mass per unit mass of fuel
C	12	7.42	89.04	0.89
H	1	3	3	0.03
S	32	0.003125	0.1	0.001
O	16	$0.375 + 0.42a(1+x)$	$6 + 6.72a(1+x)$	$0.06 + 0.0672a(1+x)$
N	14	$0.05 + 1.58a(1+x)$	$0.7 + 22.12a(1+x)$	$0.007 + 0.2212a(1+x)$
Ash	1	1.2	1.2	0.012

**Table 3 Analysis of products for  $x$  – fraction of excess air**

Products	Atomic mass	Amt of sub per 100Kg fuel	Mass per 100Kg of fuel	Mass per unit mass of of fu
CO <sub>2</sub>	44	$b = 7.42$	326.48	3.26
H <sub>2</sub> O	18	$d = 1.5$	27	0.27

SO <sub>2</sub>	64	$e = 0.003125$	0.20	0.002
O <sub>2</sub>	32	$0.21ax$	$6.72ax$	$0.0672ax$
N <sub>2</sub>	28	$0.025 + 0.79a(1 + x)$	$0.7 + 22.12a(1 + x)$	$0.007 + 0.2212a(1 + x)$
Ash	1	1.2	1.2	0.012

### 3.3.2 Flue Gas Analysis

The analysis of flue gases of combustion by masses of constituents per unit mass of fuel are carried out on wet and dry bases and recorded in Tables 4 and 5.

*Table 4 Analysis of flue gases on wet basis*

Flue gases	Mass per unit mass of fuel	Percentage weight on wet basis
CO <sub>2</sub>	3.26	$\frac{3.26}{3.539(1 + 0.0625a + 0.0815ax)}$
H <sub>2</sub> O	0.27	$\frac{0.27}{3.539(1 + 0.0625a + 0.0815ax)}$
SO <sub>2</sub>	0.002	$\frac{0.002}{3.539(1 + 0.0625a + 0.0815ax)}$
O <sub>2</sub>	$0.0672ax$	$\frac{0.0672ax}{3.539(1 + 0.0625a + 0.0815ax)}$
N <sub>2</sub>	$0.007 + 0.2212a(1 + x)$	$\frac{0.007 + 0.2212a(1 + x)}{3.539(1 + 0.0625a + 0.0815ax)}$
Total	$3.539(1 + 0.0625a + 0.0815ax)$	100

*Table 5 Analysis of flue gases on dry basis*

Flue gas	Mass per unit mass of fuel	Percentage weight on dry basis
CO <sub>2</sub>	3.26	$\frac{3.26}{3.269(1 + 0.0625a + 0.0815ax)}$
H <sub>2</sub> O	-	-
SO <sub>2</sub>	0.002	$\frac{0.002}{3.269(1 + 0.0625a + 0.0815ax)}$

O <sub>2</sub>	0.0672ax	$\frac{0.0672ax}{3.269(1 + 0.0625a + 0.0815ax)}$
N <sub>2</sub>	0.007 + 0.2212a(1 + x)	$\frac{0.007 + 0.2212a(1 + x)}{3.269(1 + 0.0625a + 0.0815ax)}$
Total	3.269(1 + 0.0625a + 0.0815ax)	100

### 3.3.3 Determination of Adiabatic flame temperature

The temperature that would be achieved by the products in the limit of adiabatic operation of a reactor or combustion system is called *the adiabatic flame temperature or adiabatic combustion temperature*. The adiabatic flame temperature,  $T_{ad}$  of the fuel in the combustion zone of the furnace is determined by employing the steady state flow energy equation in the combustion chamber while neglecting potential and kinetic energy changes. The energy equation is given by:

$$\sum_{in} MH - \sum_{out} MH = 0 \quad (7)$$

M and H are the mass and enthalpy of fuel which is represented as heat released, given by [10] as:

$$Q = H_{P2} - H_{R1} = 0 \quad (8)$$

Where  $Q$  is the heat energy,  $H_{P2}$  represents the total enthalpy of the products of combustion, and  $H_{R1}$  represents the total enthalpy of reactants.

Expanding equation (3.8), we have

$$H_{P2} - H_{R1} = (H_{P2} - H_{P0}) + (H_{P0} - H_{R0}) + (H_{R0} - H_{R1}) = 0 \quad (9)$$

$H_{R0}$  and  $H_{P0}$  are enthalpies of reactants and products at reference temperature,  $T_0$

This is rewritten as;

$$(H_{P2} - H_{P0}) + \Delta H_0 + (H_{R0} - H_{R1}) = 0 \quad (10)$$

Where  $\Delta H_0 = (H_{P0} - H_{R0})$  is the enthalpy of combustion at reference temperature,  $T_0$

The enthalpy changes may be written for an ideal gas approximately as;

$$(H_{P2} - H_{P0}) = \sum_P M_i C p_i (T_2 - T_0) \quad (11)$$

$$\text{and} \quad (H_{R0} - H_{R1}) = \sum_R M_i C p_i (T_0 - T_1) \quad (12)$$

Where  $M_i$  and  $C p_i$  are masses and specific heat capacities of reactants and products.  $T_0, T_1, T_2$  are reference, initial and final temperatures respectively.

Substituting these in equation (3.10) follows that

$$\sum_P m_i C p_i (T_2 - T_0) + \Delta H_0 + \sum_R m_i C p_i (T_0 - T_1) = 0 \quad (13)$$

Hence, the final temperature,  $T_2$  which is the adiabatic flame temperature,  $T_{ad}$  is calculated thus

$$T_2 = T_0 - \frac{\Delta H_0 - (T_0 - T_1) \sum_R M_i C p_i}{\sum_P M_i C p_i} \quad (14)$$

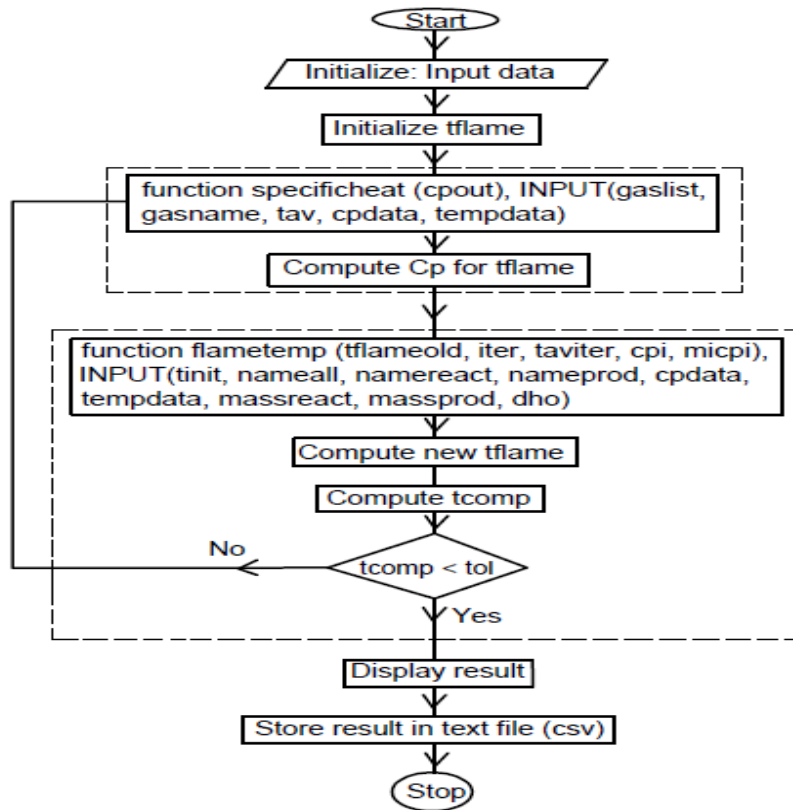
The ambient temperature is used as the reference temperature,  $T_0$  and the values of  $M_i$  and  $C p_i$  are read from Table 3 and 6.

The absolute value of the enthalpy of combustion,  $|\Delta H_0|$  for the fuel is the heating value (calorific value) of the fuel [7, 10]. Coke has a calorific value ranging from 28,000 kJ/kg to 31,500 kJ/kg [30], therefore choosing a value of 30,500 kJ/kg which is given as lower heating value (LHV) of coke [15] gives an enthalpy of combustion equal to 30,500 kJ/kg.

## Results and discussion

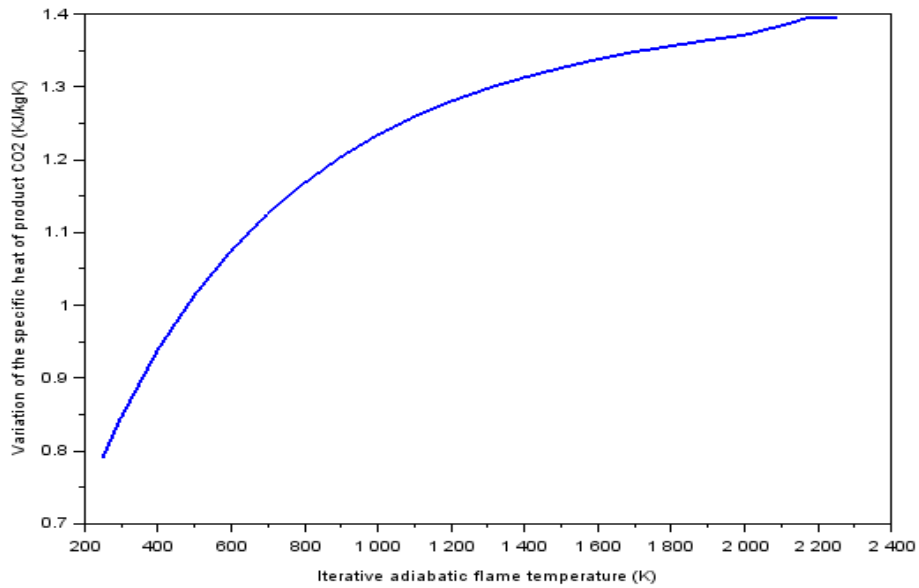
The calculations in this work which include the determination of adiabatic flame temperature, solution to the energy balance equations and the parametric study were carried out with the high performance matrix-based software, SCILAB (version 6.0.0). SCILAB is a programming language associated with a rich collection of numerical algorithms covering many aspects of scientific computing problems.

The flow charts for the SCILAB computation are presented in Figures 4

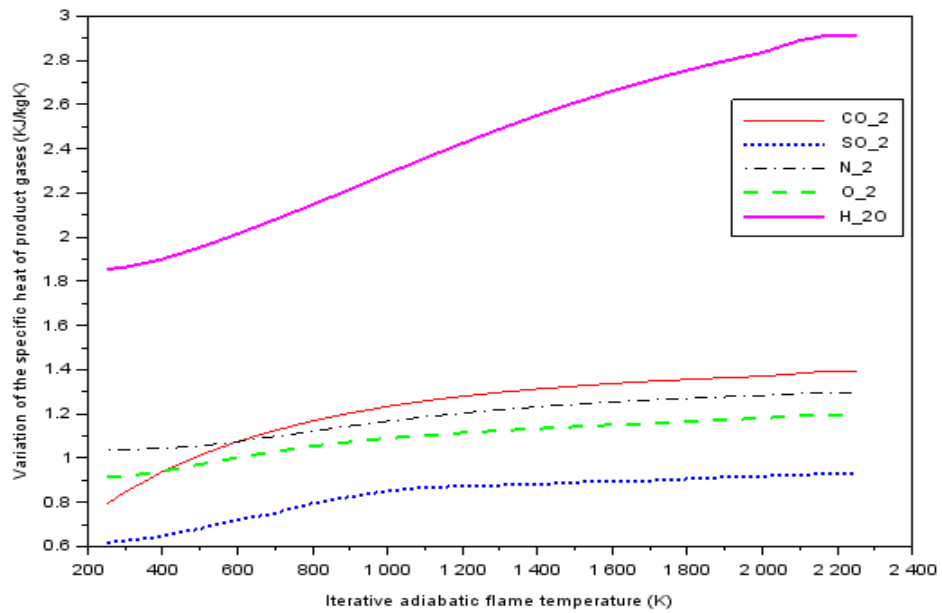


*Fig. 4 Flow chart for SCILAB computation of adiabatic flame temperature*

The adiabatic flame temperature of the fuel (coke) used in the furnace was determined by an iterative procedure with an initial value of 1000 K assumed, and the intermediate values of the specific heat of various gases were calculated by interpolation. The procedure converged at the 8<sup>th</sup> iteration, and a constant value of  $T_2$  was obtained, giving an adiabatic combustion temperature ( $T_2$ ) equal to 2175.93K as shown in Fig. 5 and Fig 6. The specific heat ( $C_p$ ) of the products keep increasing with increasing temperature from the initial guess value until the value of 2175.93K. After this temperature, there was no appreciable change in the specific heat ( $C_p$ ) of  $CO_2$  and the other products. The ash has no contribution in the combustion process and so was not necessarily captured in this analysis.



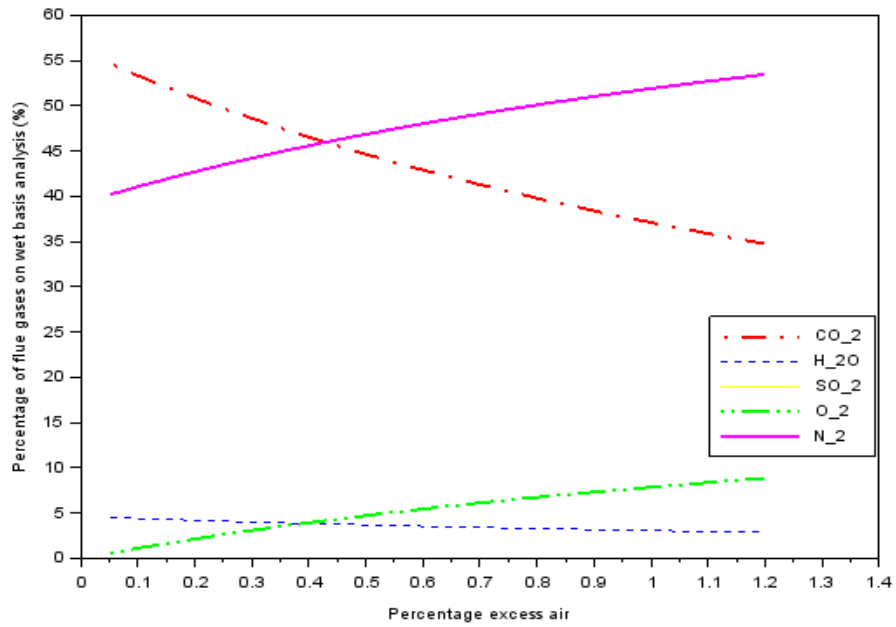
**Fig. 5: Effect of adiabatic flame temperature on CO<sub>2</sub> specific heat**



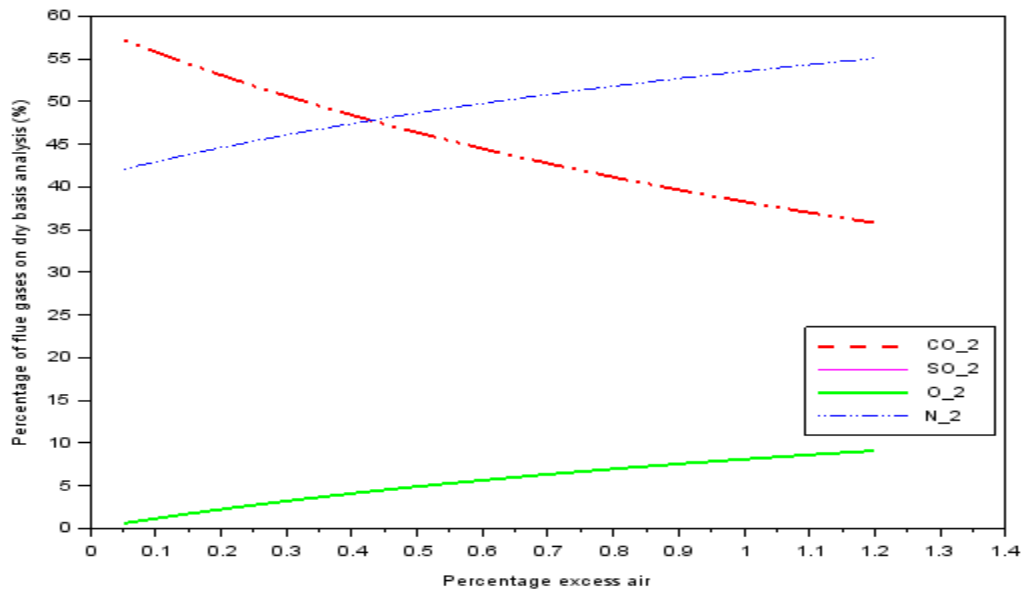
**Fig. 6: Effect of adiabatic flame temperature on gas specific heat**

This temperature is in range with adiabatic flame temperatures recorded for coke at initial temperature of 293K to be 2142K [34]. The operating temperature was assume to be constant to test the effect of

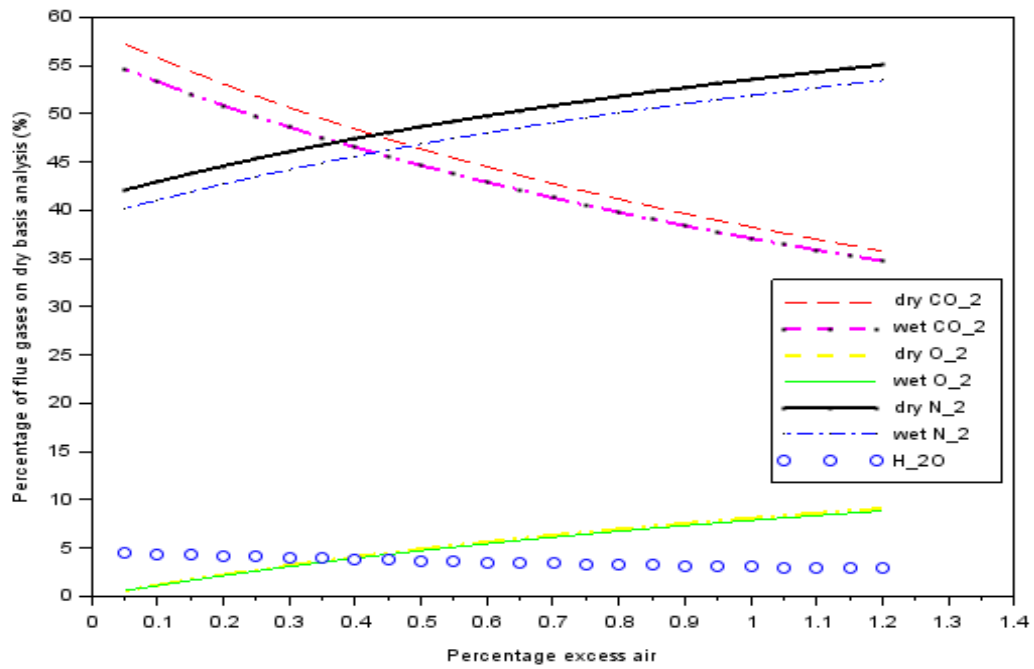
the different excess air on the flue gases both on wet and dry analysis basis from the already generated models as shown in Fig 7 and Fig 8 respectively. The percentage excess air was varied from 0.05 (5%) to 1.2 (120%) to determine their effects on the Cp of the gases considering both wet and dry basis analysis. It was discovered that the Cp of water remain almost constant at all level of percentage excess air with just differential change. That of CO<sub>2</sub> and N<sub>2</sub> shown decreasing and increasing trend respectively as the percentage excess air increase. Both intercepted at 0.43 (43%) excess air. The behavior of oxygen and water vapour from the combustion also shows the same trend but had their intercept at 0.39 (39%) excess air. The percentage composition of SO<sub>2</sub> in the combustion is comparatively infinitesimal as it within 0.0005 (0.05%) to 0.001 (0.1%) hence did not reflect on the plot. From the dry basis analysis of the flue gases percentage shown in Fig. 8, it can be seen that similar behavior occurred for their interception at exactly 0.45 (45%) whereas O<sub>2</sub> had same behavior with little increase compared to the wet analysis case. The combine effects on both wet and dry analysis case can be shown in Fig. 9 to as well see the percentage of flue gases difference for wet and dry case on different percentage excess air. The percentage of flue gases difference for wet and dry case was plotted against the percentage excess air as shown in Fig. 10. The N<sub>2</sub> and CO<sub>2</sub> curves intercepted at the point of 0.44 (44%) on the graph. This implies that the maximum of 45% (with range of 30% - 45%) excess air is required for the real balanced combustion in the furnace to give the system specified output without the dissociation of the gases and as well as the system's metallurgical consideration. Excess air above this can result to drop of the system's recommended output and possibly leads to dissociation of the products.



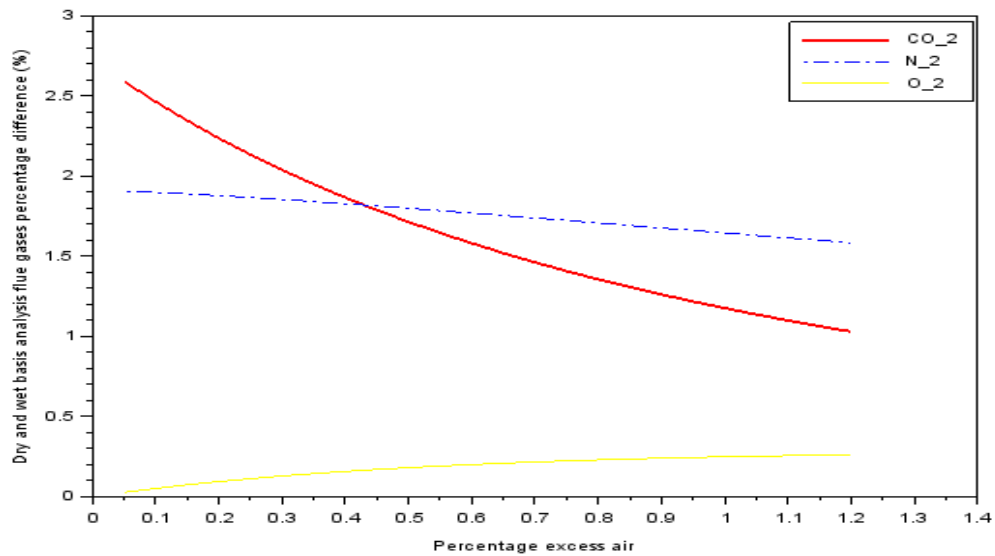
*Fig. 7: Effect of percentage excess air flue gases on wet basis analysis*



*Fig. 8: Effect of percentage excess air flue gases on dry basis analysis*



**Fig. 9: Effect of percentage excess air flue gases on both dry and wet basis analysis**



**Fig. 10 Dry and wet basis analysis flue gases percentage difference on different percentage excess air.**

## Summary

In this study, the thermal analysis of a conventional cupola furnace at the Nigeria Railway Corporation, Enugu District was carried out. The efficiency of the furnace was calculated and a parametric study was carried out to simulate possible design and operating variations for improvement of the furnace efficiency. The adiabatic flame temperature of the fuel (coke) used for operation was calculated to be 2175.93K, a high temperature value that cannot be easily controlled. Performance variations of the system was evaluated with variation of design and operating parameters. The operating parameters used were the flue gas temperature and combustion percentage excess air. The percentage excess air was varied from 0.05 (5%) to 1.2 (120%) to determine their effects on the Cp of the gases considering both wet and dry basis analysis. That of CO<sub>2</sub> and N<sub>2</sub> shown decreasing and increasing trend respectively as the percentage excess air increase. Both intercepted at 0.43 (43%) excess air. The behavior of oxygen and water vapour from the combustion also shows the same trend but had their intercept at 0.39 (39%) excess air. The percentage of flue gases difference for wet and dry case was also investigated against the percentage excess air. The N<sub>2</sub> and CO<sub>2</sub> curves intercepted at the point of 0.44 (44%). This implies that the maximum of 45% (with range of 30% - 45%) excess air is required for the real balanced combustion in the furnace to give the system specified output without the dissociation of the gases and as well as the system's metallurgical consideration.

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**Appendix A.  
Input Data**

Table 6  
*Specific heat of gases*

<b>T (K)</b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub>O</b>	<b>O<sub>2</sub></b>	<b>N<sub>2</sub></b>	<b>SO<sub>2</sub></b>
250	0.791	1.855	0.913	1.039	0.619
298	0.845	1.864	0.917	1.039	0.623
300	0.846	1.864	0.918	1.040	0.625
400	0.939	1.901	0.941	1.044	0.647
500	1.014	1.954	0.972	1.056	0.681
600	1.075	2.015	1.003	1.075	0.722
700	1.126	2.080	1.031	1.098	0.751
800	1.168	2.147	1.054	1.122	0.796
900	1.204	2.217	1.074	1.146	0.825
1000	1.234	2.288	1.090	1.167	0.851
1100	1.259	2.358	1.103	1.187	0.868
1200	1.280	2.425	1.115	1.204	0.873
1300	1.298	2.490	1.125	1.219	0.878
1400	1.313	2.552	1.134	1.232	0.882
1500	1.326	2.609	1.143	1.244	0.891
1600	1.338	2.662	1.151	1.254	0.896
1700	1.348	2.711	1.158	1.263	0.898
1800	1.356	2.756	1.166	1.271	0.906
1900	1.364	2.798	1.173	1.278	0.914
2000	1.371	2.836	1.181	1.284	0.919

2100	1.384	2.891	1.192	1.292	0.924
2175	1.395	2.915	1.198	1.298	0.930
2200	1.394	2.915	1.196	1.298	0.928
2250	1.395	2.913	1.198	1.297	0.929

## SCILAB Source Codes

### Calculation of Adiabatic Flame Temperature

```

0001 //Determination of adiabatic flame temperature
0002 //Requires user-defined functions flametemp and specifichat
0003 //myfile is the filename
0004 //mydir is the directory pathname
0005 filename = "Temp_AD.sce"
0006 filenamebase = basename(filename);//basename of current file
0007 mydir = get_absolute_file_path(filename);//get the absolute file path
0008 genlib("mylib", mydir);//generate a library of functions in this directory
0009 b = 7.42;// Number of moles of CO2 in the products
0010 d = 1.5;// Number of moles of H2O in the products
0011 a = 38.03;// Number of moles of air per 100kg of fuel
0012 raf = 10.97;// Air/fuel ratio(stoic)
0013 ex = 0.1;// Fraction of excess air used
0014 raf2 = raf * (1+ex);// Actual air fuel ratio employed
0015 xc = 7.42;// Amount of substance for Carbon (C) per 100kg of fuel
0016 xh = 3;// Amount of substance for Hydrogen (H) per 100kg of fuel
0017 xs = 0.003125;// Amount of substance for Sulphur (S) per 100kg of fuel
0018 xo = 17.94;// Amount of substance for Oxygen (O) per 100kg of fuel
0019 xn = 66.15;// Amount of substance for Nitrogen (N) per 100kg of fuel
0020 xash = 1.2;// Amount of substance for Ash per 100kg of fuel
0021 atomsr(:,2) = [b xh xs xo xn xash]';// Compute values
0022 atomicnumber = [12 1 32 16 14 1]';// Atomic number of C, H, S, O, N & Ash respectively

```

```

0023 atomsr(:,1) = atomicnumber;// Assign to column 2
0024 atomsr(:,3) = atomsr(:,1) .* atomsr(:,2);// Mass of reactants per 100kg of fuel
0025 atomsr(:,4) = atomsr(:,3)/100;// Mass of reactants per unit mass of fuel
0026 atomsrtext = ["C" "H" "S" "O" "N" "Ash"];// Reactants
0027 reactanthead = ["Reactant" "Atomic mass" "Coefficient" "Amount of substanceper 100 kg of
fuel" "Mass per 100 kg of fuel" "Mass per unit mass of fuel"];// Header for reactant table
0028 coefficient = ["89/12" "3" "0.1/32" "6/16" "0.7/14" "1.2"];// Coefficients of C, H, S, O, N and
Ash respectively in the reactants
0029 reactant = [reactanthead; atomsrtext string(atomsr(:,1)) coefficient string(atomsr(:,2:4))];//
Arrange output in columns
0030 myfile = mydir + "/" + filenamebase + "-reactant.csv"; csvWrite(reactant, myfile);//Output
filename
0031 ee = xn/2;// Number of moles of Nitrogen (N2) in the products per 100kg of fuel
0032 xo2 = 0.21 * a * ex;// Number of moles of Oxygen (O2) in the product per 100kg of fuel
0033 coeffp = ["b" "d" "xs" "xo2" "ee" "1.2"];// Amount of substance for CO2, H2O, SO2, O2, N2
and Ash in the products with excess air
0034 nameprod = ["CO2" "H2O" "SO2" "O2" "N2" "Ash"];// Combustion products name for use in
determination of specific heat as a function of temperature
0035 atomsp(:,2) = [b d xs xo2 ee xash]);// Get numerical values
0036 prodhead = ["Product" "Molar mass" "Coefficient" "Amount of subatanceper 100 kg of fuel"
"Mass per 100 kg of fuel" "Mass per unit mass of fuel"];// Header for output of product data
0037 molarmass = [44 18 64 32 28 1];// Molar mass of the products
0038 atomsp(:,1) = molarmass;
0039 atomsp(:,3) = atomsp(:,1) .* atomsp(:,2);// Mass of products per 100 kg of fuel
0040 atomsp(:,4) = atomsp(:,3)/100;// Mass of products per unit mass of fuel
0041 product = [prodhead; nameprod string(atomsp(:,2)) coeffp string(atomsp(:,2:4))];// Arrange
output data as a string
0042 myfile = mydir + "/" + filenamebase + "-product.csv"; csvWrite(product, myfile);//Output
filename
0043 namereact = atomsrtext;// Name of reactants
0044 nameall = [nameprod namereact];// List of all reactants and products

```

```

0045 cpdata = [0.845 1.234 1.338;// CO2
0046         1.864 2.288 2.662;// H2O
0047         0.623 0.851 0.896;// SO2
0048         0.917 1.090 1.151;// O2
0049         1.039 1.167 1.254;// N2
0050         0.71 0.71 0.71;// Ash
0051         0.71 0.71 0.71;// fuel
0052         1.039 1.167 1.254;// Air, assumed same as that of N2
0053     ];           // Specific heat of each products at 298, 1000 and 1600 Kelvin respectively
0054 tempdata = [298 1000 1600];// Temperature at which the cps are specified
0055 t_o = 298;// Reference temperature
0056 treact = t_o;// Initial temperature of reactants
0057 t2 = 1000;// Initial estimate of adiabatic flame temperature
0058 tinit = [treact t_o t2]
0059 tol = 1 * 10(-4);// Tolerance
0060 t2x = [t2];// Initialise
0061 change = 1000;
0062 dho = -30500;// Enthalpy of combustion in kJ per kg
0063 massreact = [1 raf2]);// Mass of reactants per unit mass of fuel
0064 massprod = atomsp(:,4);// Mass of products per unit mass of fuel
0065 [tflameold, iter, taviter, cpi,micpi] = flametemp(tinit,nameall,namereact, nameprod, cpdata,
tempdata, massreact,massprod,dho) //Calculate adiabatic flame temperature. All temps are in degree
Kelvin
0066 disp(t2x);// Display the calculated values
0067 result = [[1:iter-1] tflameold(2:$) taviter cpi]);// Output data
0068 Heading = ["Iteration No" "T_ad (K)" "T_av (K)" "CO2" "H2O" "SO2" "O2" "N2" "Ash"];
0069 resultout = [Heading; string(result)];
0070 myfile = mydir + "/" + filenamebase + "-iteration.csv"; csvWrite(resultout, myfile);//Output
filename

```