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# Computer Programming for Estimation of Temperature of Combustion Products and Cost Comparison of Different Coals

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## Abstract

Coal, being a complex fuel difficult to analyze when it comes to evaluate the comparative offers of coals. Moreover the fact that, most of the time, apparatus for ultimate analysis is not available makes this job even more difficult. Computer programming is employed in order to address this issue and this paper provides an insight of the software developed.

The determination of the flame temperature involves tedious calculations which are to be carried out quite regularly for handling coal firing furnaces. Software developed for this purpose makes this process a lot more convenient as the input data mainly comprises of proximate analysis which can easily be determined. Following pages reflect upon the methodology adopted and the functioning of software.

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## Introduction

The renaissance of coal usage has revolutionized the economics of coal technology. The competitive market has optimized the cost effectiveness of coal combustion systems in the near past. These recent developments along with innovative coal testing equipment have eased the technical analysis of coals and it is inevitable to analyze coal on the basis of intended consumption requirements.

The cost of coal is usually available on the basis of weight i.e. Rupees per ton or Dollars per ton and not on the basis of heating value. This might lead to the wrong selection of coal. The prime reason is the difference between gross and net calorific value of coal which are defined as

### Gross calorific value (GCV)(2)

Gross calorific value or higher heating value is the quantity of heat liberated by combusting the fuel at a constant volume in oxygen saturated with water vapor, the original material and final products of combustion being at a reference temperature and the water obtained in the flue gas being in the liquid state.

### Net Calorific Value (NCV)

Net Calorific Value or lower heating value at a constant volume is the quantity of heat evolved when the when unit quantity of fuel is burnt at a constant volume in oxygen saturated with water vapor, the original material and final products of combustion being at a reference temperature and the water obtained in the flue gas being in the vapor state.

The hydrogen present in coal is usually associated with volatile matter (2). This Hydrogen combines with oxygen and gets converted into water vapor, which liberate the heat as by other exothermic combustion reactions. The net useful heat however, is less than the gross heating value of the coal by the amount corresponding to the heat of condensation of water vapors.

Formula of Net Calorific Value is

$$NCV = GCV - m\lambda$$

Where $m$ = mass of water formed

$\lambda$ = Latent Heat of Vaporization of water at $25^{o}$C.

The water in the flue gas includes the water formed by the oxidation of hydrogen present in coal as well as the external moisture.

## Temperature of combustion products

Temperature of combustion products can be determined both theoretically and experimentally. In order to determine the theoretical temperature a series of calculations is necessary. Computer programming may help in this context and the developed software utilizes the proximate analysis of the coal, which is readily available.

The estimation of the theoretical temperature of the combustion product will help in furnace design/ operation. Moreover it can be helpful whenever coal firing equipment is designed. The software provides a readily available tool to measure the theoretical temperature of combustion products quite easily.

The combustion reactions considered are

$C + O_2 = CO_2$
$H_2 + \frac{1}{2} O_2 = H_2O$
$S + O_2 = SO_2$

The temperature of the combustion products can be observed from the graph formed. At the Point on the straight line where the values of calculated and assumed temperature are equal, that gives the temperature of the combustion products. The value of assumed temperature will be taken as the result with the equivalent calculated temperature value.

## Experimental Work

The experimental work was carried out on the PMDC Degyari coal sample.

The results obtained were as under

| Sr. No. | Test Name | Result (Percentage) |
|---|---|---|
| 1 | Air Dry Loss | 4.61 |
| 2 | Inherent Moisture | 7.67 |
| 3 | Volatile Matter | 41.99 |
| 4 | Ash | 8.43 |
| 5 | Fixed carbon | 37.33 |
| 6 | Sulfur | 4.90 |
| 7 | Gross Calorific Value (Kcal/Kg) | 6158 |
| 8 | Hard Groove index | 39 |

Software for the Comparison of the cost of different coals requires input data in the following format

| Evaluation of offers for coal | | |
|---|---|---|
| **Parameters** | **PMDC Degyari** | **Coal 2** |
| Total Moisture %(ARB) | 12.28 | 15.00 |
| Volatile Matter %(As Received Basis) | 41.99 | 34.00 |
| Gross Calorific Value (As Received Basis) | 6158.00 | 6290.00 |
| Price Rupees per ton | 4800.00 | 6500.00 |

The resultant output is obtained as under

| Calculations | | |
|---|---|---|
| Hydrogen % (ARB) | 4.29 | 3.83 |
| N .C .V (K.cal/Kg) | 5860.98 | 6001.16 |
| Cost of coal/Kg (Rs) | 4.80 | 6.50 |
| Coal consumption(Kg) to transfer 10,000 Kcal Heat | 1.71 | 1.67 |

| | | |
|---|---|---|
| **Cost per 10,000 Kcal Heat (Rs)** | **8.19** | **10.83** |

Formulation operating at the backend of the software is as follows.

| **Calculations** | |
|---|---|
| Hydrogen % (ARB) (4) | =(0.069*( (Gross Calorific Value) /100+ (Volatile Matter))-2.86) |
| N .C .V (K.cal/Kg) | = Gross Calorific Value -((0.0894* Hydrogen)+( Total Moisture /100))*587 |
| Cost of coal/Kg (Rs) | = Price per ton /1000 |
| Coal consumption(Kg) to transfer 10,000 Kcal Heat | =10000/ N .C .V. |
| **Cost per 10,000 Kcal Heat (Rs)** | **=** (Coal consumption(Kg) to transfer 10,000 Kcal Heat) x (Cost of coal/Kg) |

## Temperature of Combustion Products

The software developed for the determination of theoretical temperature of combustion products has input data as under

| **Percentage Composition** | |
|---|---|
| **Proximate Analysis** | |
| Ash % | 8.43 |
| $H_2O$ % | 12.28 |
| Volatile Matter % | 41.99 |
| Fixed Carbon % | 37.33 |
| G.C.V (KCal/Kg) | 6158.00 |
| Sulfur | 4.90 |
| Excess Air % | 10.00 |
| Temp of Air Supplied °C | 25.00 |

The output is obtained as under

| **Derived Ultimate Analysis (%) excluding ash and water** | |
|---|---|
| C | 56.01 |
| H | 3.40 |
| N | 1.50 |
| S | 3.89 |
| $O_2$ | 14.50 |

| **Solution** |
|---|
| Basis 100 Kg Coal as Fired |

| | |
|---|---|
| Total heat Available(KJ/Kg Coal) | 21535.60 |
| Mean Specific Heat of Combustion Products (KJ/Kg. deg C) | |

| **Calculations for Kg Moles** | **Kg-Moles** |
|---|---|
| C | 4.67 |
| $H_2$ | 1.70 |
| N | 0.05 |
| S | 0.12 |
| $O_2$ | 0.45 |
| $H_2O$ | 0.68 |

| | |
|---|---|
| At 1700 °C | 1.2251 |
| At 1800 °C | 1.2313 |
| At 1900 °C | 1.2366 |
| At 2000 °C | 1.2454 |
| At 2100 °C | 1.2516 |
| At 2200 °C | 1.2565 |
| At 2300 °C | 1.2657 |

The remaining calculations appear are as under

| **Solution** | |
|---|---|
| Basis 100 Kg Coal as Fired | |
| **Calculations for Kg Moles** | **Kg-Moles** |
| C | 4.67 |
| $H_2$ | 1.70 |
| N | 0.05 |
| S | 0.12 |
| $O_2$ | 0.45 |
| $H_2O$ | 0.68 |
| | |
| **Calculations of Air Supplied** | **Kg-Moles** |
| Theoretical O2 Required | 5.19 |
| Theoretical Air Required | 24.69 |
| Excess air supplied | 2.47 |
| Total Air | 27.16 |
| | |
| **Combustion Products** | **Kg** |
| $CO_2$ | 205.37 |
| $H_20$ | 42.87 |
| $N_2$ | 602.34 |
| $SO_2$ | 7.77 |
| $O_2$ | 16.59 |
| **Total Flue Gas** | 874.95 |
| | |
| **Net Calorific Value (Kcal)** | 5106.03 |
| **Net Calorific Value(KJ/Kg Coal)** | 21338.09 |
| Cp of air at 25°C(Kcal/Kg°C) | 0.24 |
| Sensible heat in air at 25°C (Kcal) | 47.26 |
| Sensible heat in air at 25°C (KJ) | 197.51 |

| Total heat Available(KJ/Kg Coal) | 21535.60 |
|---|---|
| Mean Specific Heat of Combustion Products (KJ/Kg. deg C) | |
| At 1700 °C | 1.2251 |
| At 1800 °C | 1.2313 |
| At 1900 °C | 1.2366 |
| At 2000 °C | 1.2454 |
| At 2100 °C | 1.2516 |
| At 2200 °C | 1.2565 |
| At 2300 °C | 1.2657 |
| | |
| Temperatures | |
| **Assumed** | **Computed** |
| At 1700 °C | 2009.08 |
| At 1800 °C | 1998.92 |
| At 1900 °C | 1990.44 |
| At 2000 °C | 1976.34 |
| At 2100 °C | 1966.64 |
| At 2200 °C | 1958.87 |
| At 2300 °C | 1944.59 |
| Mass Fractions of Combustion Products | |
| $CO_2$ | 0.23 |
| $H_20$ | 0.05 |
| $N_2$ | 0.69 |
| $SO_2$ | 0.01 |
| $O_2$ | 0.02 |

The formulation used for the derived ultimate analysis is as under

| Derived Ultimate Analysis | |
|---|---|
| C | = 0.59 x [(G.C.V / 100)- (0.369x VM] + 43.4 |
| H | = 0.069 x [(G.C.V / 100)+VM] – 2.86 |
| N | = average value of nitrogen generally present in bituminous coal |
| S | Measured by XRF |
| $O_2$ | = By difference |

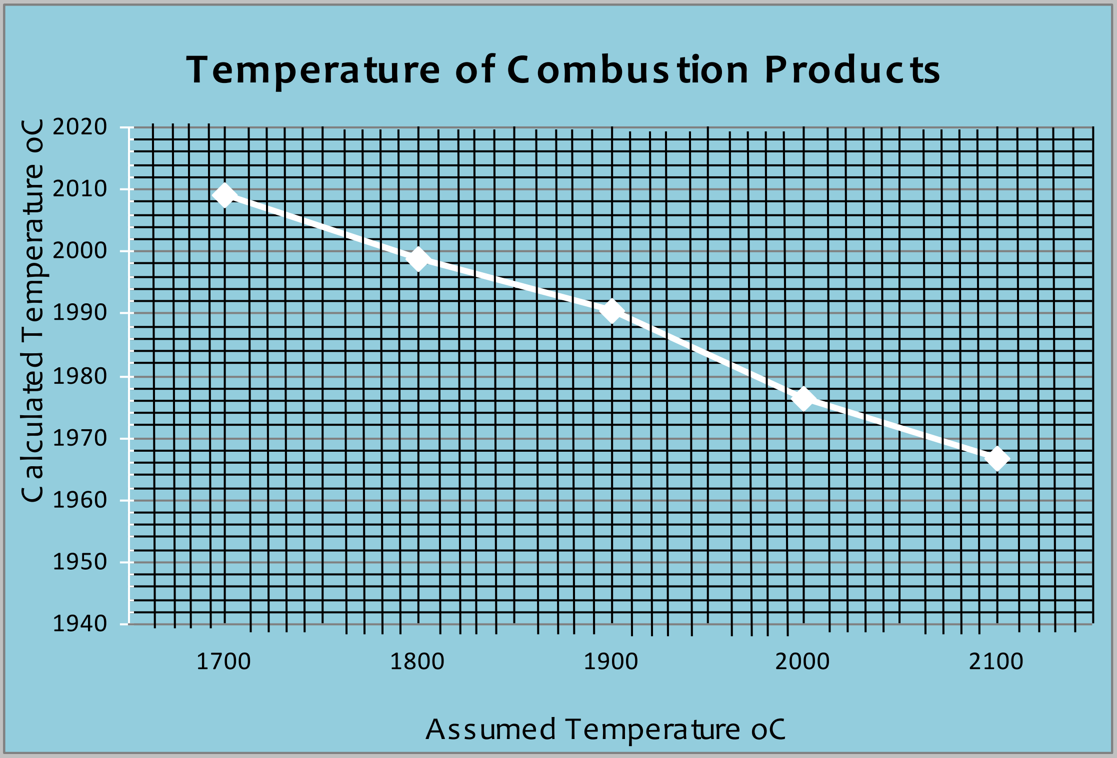
The formulation used for the calculations is

| **Solution** | |
|---|---|
| Basis 100 Kg Coal as Fired | |
| **Calculations for Kg Moles** | **Kg-Moles** |
| C | = %age of C/12 |
| H2 | = %age of $H_2$/2 |
| N | = %age of N/28 |
| S | = %age of S/32 |
| O2 | = %age of $O_2$/32 |
| H2O | = %age of $H_2O$/18 |
| **Calculations of Air Supplied** | **Kg-Moles** |
| Theoretical $O_2$ Required | = K-Mol of C + (K-Mol of $H_2$)/2 + (K-Mol of S) - K-Mol of (K-Mol of $O_2$) |
| Theoretical Air Required | = Theoretical $O_2$ Required x (100/21) |
| Excess air supplied | = Theoretical Air Required x (%age of excess air/100) |
| Total Air | = Theoretical Air Required + Excess air supplied |
| **Combustion Products** | **Kg** |
| $CO_2$ | = K-Mol of $CO_2$ x 44 |
| $H_20$ | = (K-Mol of $H_2O$ formed + K-Mol of Coal Moisture) x 18 |
| N | =((K-Mol of N present in coal) + (K-Mol of N from air)) x28 |
| $SO_2$ | = K-Mol of $SO_2$ Formed x 64 |
| $O_2$ | = (K-Mol of $O_2$ from excess air ) x 32 |
| **Total Flue Gas** | =Sum of the above |
| **Net Calorific Value(Kcal)** | = GCV-((Kg of water in combustion products /100)*2454) |
| **Net Calorific Value(KJ/kg coal)** | = Net Calorific Value(Kcal) x 4179/1000 |
| Cp of air at $25^{O}C(Kcal/Kg^{o}C)$ | 0.24 |
| Sensible heat in air at $25^{O}C$ (Kcal) | =( Total Air x 29/100) x Cp of air at $25^{O}C(Kcal/Kg^{o}C)$ x (Temp of Air Supplied) |
| Sensible heat in air at $25^{O}C$ (KJ) | = Sensible heat in air at $25^{O}C$ (Kcal) x 4179/1000 |
| Total heat Available(KJ/Kg Coal) | =(Sensible heat in air at $25^{O}C$ (KJ)) + (Net Calorific Value(KJ/kg coal)) |
| Mean Specific Heat of Combustion Products (KJ/ Kg.deg C)(3) | |

| | |
|---|---|
| At 1700 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 1700$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 1700$^{o}$C )+ (Mass Fraction of N x Cp Of N at 1700$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 1700$^{o}$C )) x 4179/1000 |
| At 1800 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 1800$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 1800$^{o}$C )+ (Mass Fraction of N x Cp Of N at 1800$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 1800$^{o}$C )) x 4179/1000 |
| At 1900 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 1900$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 1900$^{o}$C )+ (Mass Fraction of N x Cp Of N at 1900$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 1900$^{o}$C )) x 4179/1000 |
| At 2000 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 2000$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 2000$^{o}$C )+ (Mass Fraction of N x Cp Of N at 2000$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 2000$^{o}$C )) x 4179/1000 |
| At 2100 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 2100$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 2100$^{o}$C )+ (Mass Fraction of N x Cp Of N at 2100$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 2100$^{o}$C )) x 4179/1000 |
| At 2200 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 2200$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 2200$^{o}$C )+ (Mass Fraction of N x Cp Of N at 2200$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 2200$^{o}$C )) x 4179/1000 |
| At 2300 $^{o}$ C | =((Mass Fraction of $CO_2$ x Cp Of $CO_2$ at 2300$^{o}$C ) +(Mass Fraction of $H_2O$ x Cp Of $H_2O$ at 2300$^{o}$C )+ (Mass Fraction of N x Cp Of N at 2300$^{o}$C )+ (Mass Fraction of $O_2$ x Cp Of $O_2$ at 2300$^{o}$C )) x 4179/1000 |

| Mass Fractions of Combustion Products | |
|---|---|
| $CO_2$ | = mass of $CO_2$ (Kg) / Total Flue gas |
| $H_20$ | = mass of $H_2O$ (Kg) / Total Flue gas |
| N | = mass of N (Kg) / Total Flue gas |
| $SO_2$ | = mass of CO (Kg) / Total Flue gas |
| $O_2$ | = mass of $O_2$ (Kg) / Total Flue gas |

| Assume Temperatures | Calculated Temperatures |
|---|---|
| At 1700 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 1700$^{o}$C) |
| At 1800 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 1800$^{o}$C) |
| At 1900 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 1900$^{o}$C) |
| At 2000 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 2000$^{o}$C) |
| At 2100 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 2100$^{o}$C) |
| At 2200 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 2200$^{o}$C) |
| At 2300 $^{o}$ C | = (Total heat Available(KJ/Kg Coal))/((Total Flue Gas /100) x (Mean Specific Heat at 2300$^{o}$C) |



The answer will be obtained by locating that point on the graph at which both the values of assumed temperature and calculated temperature are equal.

## References:

[1] Gupta OP, Fuel Furnaces and Refractories, Romesh Chandar Khana, 2003, pp 4.

[2] ---------------------IBID------------------------- ,pp 18.

[3] ---------------------IBID------------------------- ,pp *916.*

[4] Speight G J. The Chemistry and Technology of coal, Marcel dekker, INC. 1994, pp 8.