TED ANKARA COLLEGE FOUNDATION HIGH SCHOOL

IB STANDARD LEVEL CHEMISTRY EXTENDED ESSAY

COMPARISON OF THE EFFICIENCY OF DIFFERENT CARBON BASED FUELS DEPENDING ON THE AIR POLLUTANTS RELEASED PER HEAT ENERGY

Candidate's Name: Alican Salor
Candidate's Number: 001129-057
Supervisor's Name: Sedef Eryurt
Word Count: 3880 Words

Alican Salor
001129–057

Abstract

In this project the heat values and the amount of air pollutants such as oxides of sulfur, oxides of nitrogen and CO_2 released into the atmoshpere of Lignite (Soma coal), Bituminous coal (Zonguldak coal), Subbituminous coal (Beypazarı coal), Octane, Dodecane and Hexadecane are calculated and examined by using a bomb calorimeter.

The aim of this project is to compare the heat values and amount of air pollutants released into the atmosphere after the combustion of these widely used carbon based fuels. Moreover from these comparisons the most efficient carbon based fuel (depending on the amount of air pollutant released per heat energy given out) can be determined.

Throughout the experiment these fuel types are combusted in a bomb calorimeter. Through the combustion reactions the temperature of the system is observed and both the higher and lower heating values of the fuels are calculated. Moreover temperature change versus time graphs are drawn to determine how fast, intense or orderly the reactions occur. Apart from these the amounts of air pollutant released are calculated by using the combustion reaction formula of each fuel.

In the conclusion of the project it is found that Zonguldak coal has the highest heating value however it releases much more carbondioxide to the atmosphere than the other fuels. Octane on the other hand has the lowest heating value. Apart from these comparison, in order to compare the efficiency of the fuels, heating values are proportioned with the amounts of air pollutants released. When assuming only one type of air pollutant is present (only CO_2 by using control methods). From this comparison it is found that Soma coal is the most efficient fuel. However when assuming that there are no control methods present, most efficient fuel type is found to be Hexadecane.

(294 Words)

Table of Contents

Alican Salor
001129–057

Aim Of The Project

In this project the effeciency and damage caused by CO_2 and other harmful gases (oxides of sulfur and nitrogen) which are released after combustion of widely used carbon based fuels will be compared.

Research Question

Can the efficiency of widely used carbon based fuels ,such as petroleum and coal, be maximized by minimizing the amount of air pollutants (oxides of sulfur, nitrogen, carbon dioxide etc) released into the atmoshpere per amount of heat energy given out?

Introduction

   Since the industrial developments that was seen in Europe around 18th and 19th centuries, the world gradually become more dependant on the resources of energy. 'The Industrial Revolution may be defined as the application of power-driven machinery to manufacturing'[1]. So as you can see the reason for this dependancy was caused by the heart of industralisation which is the mechanised production.
   When everything became mechanical in factories, the human mistakes were decreased to minimum and the rate of production was increased as well as the profits. So we can say that production became much more efficient. However in order to make these machines work a source of energy was needed. This source of energy was heat which was obtained from the combustion reactions such as the combustion of coal. However this type of energy was valuable only when it is converted into mechanical energy. The conversion was done by the steam engine. "The development and subsequent application of steam power was undoubtedly the greatest technical achievement of the Industrial Revolution. A number of industries needed the ability to apply the enormous power produced by the steam engine, in order to continue their advancement in production."[2] So you can see how a important role carbon based fuels (mostly coal in the 18 and 19th centuries) have in the development of the industuries.
This importance still remains as most of the machines work with the same principle (mostly automobile engines) of converting heat energy obtained from a combustion reaction to mechanical energy. However now, it is a known fact that coal or petroleum, which are widely used carbon based fuels in todays world, after combustion releases carbon dioxide into the atmosphere because both "consist of a complex mixture of hydrocarbons (mostly alkanes) of various lengths"[3] and this is the greatest cause of the greenhouse effect as CO_2 is released after combustion.
   The greenhouse effect is simply this: "The earth's atmosphere is transperant to visible light from the sun. This visible light strikes the earth, and part of it is changed to infrared radiation. The infrared radiation from the earth's surface is strongly absorbed by CO_2 in

---

[1] McLamb, Eric. "The Industrial Revolution and Its Impact on Our Environment". May 19, 2008. http://www.ecology.com/archived-links/industrial-revolution/index.html
[2] Montagna, Joseph A. "The Industrial Revolution". http://www.yale.edu/ynhti/curriculum/units/1981/2/81.02.06.x.html
[3] http://en.wikipedia.org/wiki/Petroleum

the atmosphere. In effect the atmosphere traps some of the energy, acting like the glass in a greenhouse and keeping the earth warmer than it would be otherwise."[4] The aftermath of this warming is seen in the change of weather conditions and lots of other things that change the balance of the earth

What's more not only CO_2 is released into the atmosphere with the combustion of coals and other fuels. As these contain some amounts of sulfur and nitrogen, oxides of sulfur and nitrogen which are gases will be released into the atmosphere. These from acidic solution when dissolved in water. So these air pollutants apart from greenhouse effect cause acid rains and lots of other damage to the environment.

Still there is a search for other energy sources in order to stop this greenhouse effect, other harmful effects of air pollutant and as a preparation in case the energy sources used today end up. The several potential energy sources are : "the sun (solar), nuclear processes (fission and fusion), biomass (plants), and synthetic fuels. And direct use of sun's radiant energy to heat our homes and run our factories and transportation systems seems a sensible long-ternm goal"[4]

However if we look at the matter in a more realistic way we will see that there is no way countries will make radical changes in their policies on energy sources as petroleum and coal form on of the biggest cuts in their economy. So if there was a radical change from these sources to a new source of energy their economies would collapse. This is why until these sources end up they won't let a radical change to happen.

But still there are things we can do. One of them in my opinion is to find the most efficient fuel based on the energy they conserve, amount of CO_2 oxides of sulfur and nitrogen released after combustion etc. By this way we can minimize the air pollutants released into the atmosphere and maximize the efficiency of the fuels. **This is the puspose of my extended essay and I hope to get more information about this through experiments.**

Background Research

Coal

Coal is formed from the remains of plants that are buried underground and subjected to high pressure and heat over long periods of time. Plant materials have a high content of cellulose which has the empirical formula of CH_2O. So over long periods of time chemical changes gradually lower the oxygen and hydrogen content of the cellulose molecules. Through this changes, coal matures though 4 stages: lignite, subbituminous, bituminous and anthracite.

As anthracite is the most valuable coal because of its carbon content and the low amount of reservoirs present in the earth, it is really hard to find these kind of coal. So in this experiment just lignites, subbitumunious and bituminous coals (mostly present in Turkey) will be used.

---

[4] Zumdahl, Chemistry Sixth Edition, pg 270,271

Petroleum

Petroleum is a thick, dark liquid composed mostly of compunds called hydrocarbons that contain carbon and hydrogen. It still not fully understood how petroleum is produced however it is most likely formed by the remains of marine organism.
The composition of petroleum varies with different amount of hydrocarbons used and causes the formation of different kinds of petroleum

These kinds of petroleum for example are gasoline, lpg, kerosene, diesel fuel however it mostly consists of hydrocarbons having chains that contain from 5 to more than 25 carbons. These hydrocarbons (the ones that will be used in the experiment) are octane which is found in gasoline, hexadecane which is used in diesel fuel and dodecane (which is used in kerosene).

Calorimetry

"Calorimetry, simply the science of measuring heat of reactions, is based on observing the temperature change when a body absorbs or discharges energy as heat."[5] Every substance respond differently to being heated because of the nature of the elements that substance is composed of. So one substance might require more heat energy in order to raise its temperature by one degree, on the other hand another substance might raise its temperature by two degrees with the same amount of heat energy. This is called the heat capacity C of a substance. It is defined as;

$$C = \frac{heat\ absorbed}{increase\ in\ temperature}$$

This is a very important aspect in the experiment because in order to find the amount heat energy given out as combustion of fuels is a exothermic reaction we need to determine the heat capacity of the surrounding.

Calorimeters and Bomb Calorimeter

"A calorimeter is a device used in calorimetry, for measuring the heat of chemical reactions or physical changes as well as heat capacity."[5] Although calorimeter that are used for highly accurate work are precision instruments, a very simple calorimeter can help us understand the fundamentals of calorimetry. This very simple calorimeters are called "coffee-cup calorimeter" which is formed by two nested cups and a thermometer. The outer cup provides extra insulation and the inner cup holds the solution in which the reaction occurs.

As the reaction occurs there will be a increase or decrease in the temperature which can be observed from the thermometer. Moreover we know that:

---

[5] Zumdahl, Chemistry Sixth Edition, pg 250

Energy released by reaction = energy absorbed by solution
= specific heat capacity x mass of solution x increase in temperature
= s x m x ΔT

So by using this formula we can determine how much heat energy is gained by the solution.

This is the very fundamental of calorimetry, however as I will be doing an experiment based on a combustion reaction I will have to use a different calorimeter than "coffee-cup calorimeter". A bomb calorimeter is a type of calorimeter that is used in measuring the heat of combustion reactions under conditions of constant volume. Reactants are weighed and put inside the a steel container called "bomb", then ignited. After explosion as combustion is an exothermic reaction, there will be an increase in temperature of the water and other calorimeter part. The energy change can be determined by measuring this increase in temperature. As this is a constant-volume process, the change in volume ΔV is equal to zero, so work (which is $-P\Delta V$) is also equal to zero. Therefore,

"$\Delta E = q + w$
$\quad = q$ $\qquad\qquad$ (constant volume)
$\quad = q_v$"[6]

This means that:
"Energy released by the reaction
$\qquad$ = temperature increase x energy required to change the temperature by 1°C
$\qquad$ = ΔT x heat capacity of calorimeter"[7]

By using this equation we can find the heat energy released from the combustion reaction. However as you can see we need to determine the heat capacity of the calorimeter which is the combination of the heat capacity of the bomb, the water surrounding, the stirrer, the thermometer and the water container. It can simply be found by running a test using a compund whose heat of combustion is known. Mostly for this test benzoic acid is used which has the heat of combustion of 6.32 kcal/g. So now we can rearrange the equation to:

$$\text{Heat capacity of calorimeter} = \frac{\text{energy released by the reaction}}{\Delta T}$$

There are two diffrent types of heating values that can be measured by a bomb calorimeter. These are called lower heating value and higher heating value. If the water formed evaporizes while the combustion of the fuel the heating value is called lower heating value. If the water formed stays in liquid form this is called higher heating value. The difference between these values is the latent heat of evaporization. However because

[6] Zumdahl, Chemistry Sixth Edition, pg 253
[7] Zumdahl, Chemistry Sixth Edition, pg 254

this experiment is done in room conditions, the water formed from the combustion reaction condenses so, the value found is the higher heating value.

Calculation of Higher Heating Value

$$H_0 = \frac{W \, x \, (t_m + c - t_0) - b}{G}$$

H_0 : Higher heating value (cal/g)
W : Heat capacity of the calorimeter (cal/g)
 t   : The total of temperatures observed while the combustion reaction other then the initial and final temperatures(°C)
t_0 : The initial temperature of the calorimeter before combustion starts (°C)
t_m : The final temperature of the calorimeter before the combustion ends (°C)
b   : the total heat released from the combustion of metarials (wire, N, S) other then the sample

$$b = b_D + b_N + b_S$$

b_D : The heat released from the wire that is compressed in the sample. This value is 1.6 cal for 0.1 mm diameter steel wire
b_N : The heat released when the N in the sample forms N_2O_5 by combustion. This value is 1.45 cal, per 1ml of 0.1 mole HNO_3
b_S : The heat released when S forms SO_3 when combustion occurs. This value is 3.6 cal, per 1ml of 0.1 mole H_2SO_4
G   : The mass of sample dried in air
c   : Correcting factor of the heat transfer between calorimeter and environment. This factor is calculated with Regnault – Pfaundler formula:

$$c = n \, x \, m - (n + v) \, x \, F$$

$$F = m - \frac{1}{t_n - t_v} \left(t + \frac{t_0 + t_m}{2} - m \, x \, t_v \right)$$

m : The total time for combustion (min)
v   : The mean of decrease in temperature per minute in the first phase
n   : The mean of decrease in temperature per minute in the last phase
t_v : The mean of temperatures noted in first phase
t_n : The mean of temperaures noted in last phase

The F factor can be found by using the equation given above. However for every fuel under same conditions it is found that this F factor has very close values. So in practical, the values given below can be used:

F = 1.0 : if the temperature increase in first minute is higher than the temperature increase in second minute in combustion state

F = 1.25 : if the temperature increase in first minute is equal to the temperature increase in second minute in combustion state

F = 1.5 : if the temperature increase in first minute is lower than the temperature increase in second minute in combustion state

Calculation of Lower Heating Value

$$H_u = H_0 - 5.85 \, x \, (9H + K)$$
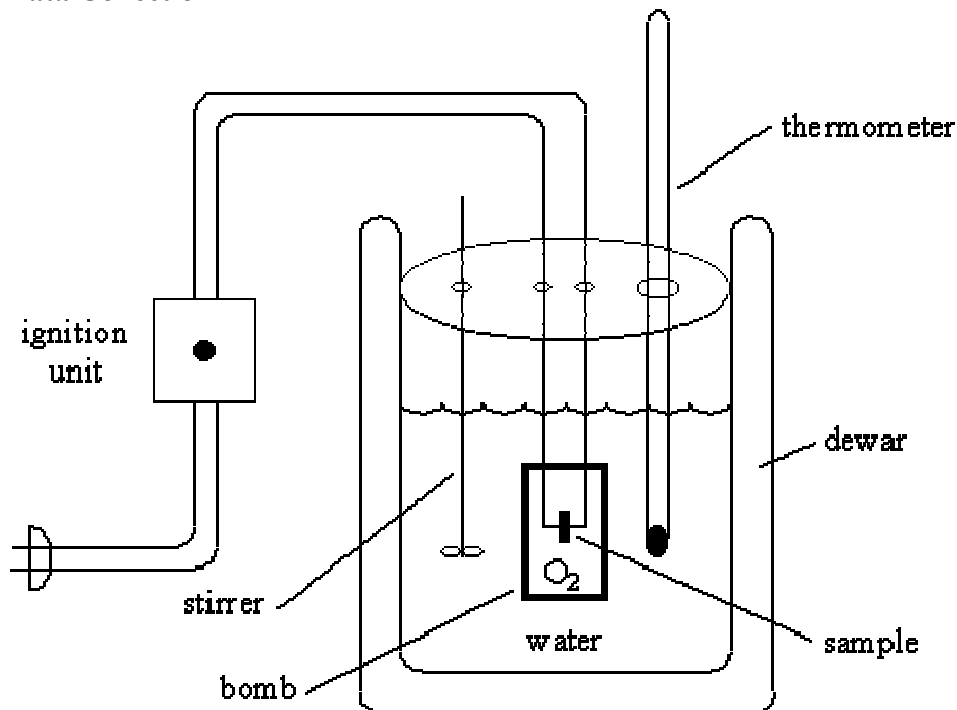
H_u : Lower heating value

H_0 : Higher heating value

H   : %H_2O amount that is in the sample fuel

K   : %moist amount that is in the sample fuel

Throughout the experiments A, B, C coal samples are used, which contain different amounts of C, H, N, S, O, moist and ash. In the experiments D, E, F liquid hydrocarbons that are mainly present in liquid fuels are used. So these samples doesn't contain O, N, S, moist or ash. And because pure O_2 is used for combustion instead of air, N_2 that is present in air is neglected too.

Data Collection

Figure 1: shows the display of the experiment

---

[8] http://www.chem.hope.edu/~polik/Chem345-2000/bombcalorimetry.htm

Alican Salor
001129–057

The apparatus used in the experiment is prepared according to the methods in Appendix 1. Finally when the apparatus is set up and ready to be started the stirrer button must be turned on. Then:

i.   The temperature change of this first phase (cooling down the system) must be noted down. This phase usually takes 6-8 minutes.

ii. In the second phase the ignition of the sample is started. A sudden temperature will be observed on the Beckmann thermometer. Approx. in 3 minutes this temperature change will reach maximum value. However this period of time changes with different samples. All the temperature changes in this phase must be noted down until the temperature stabilizes.

iii. The last phase is again the cooling down of the system. As the combustion is completed the system will start cooling down and a decrease in Beckmann thermometer will be observed. All the temperature changes must be noted down until the temperature stabilizes.

These 3 phases will be repeated in all samples and detailed information for every phase can be found in appendix 1.

Throughout the experiments the following samples are used:

- Lignite (Soma coal)
- Bituminous coal (Zonguldak coal)
- Subbituminous coal (Beypazarı coal)
- Octane
- Dodecane
- Hexadecane

The heat capacity of the calorimeter used throughout the experiment is found to be 3300 cal with benzoic acid.
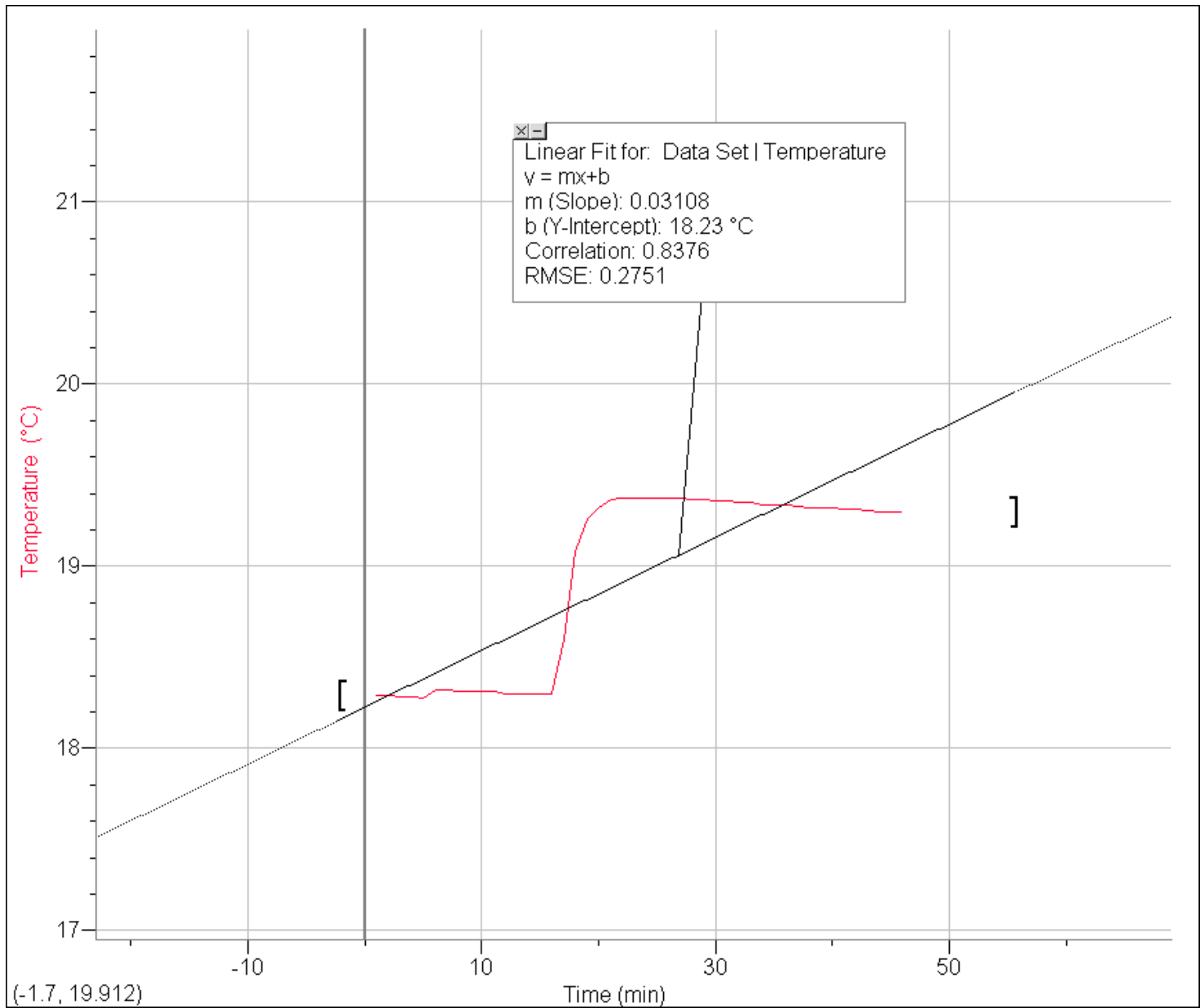
EXPERIMENT A – Bituminous coal (Zonguldak Coal)

Mass of sample with wire(gr) (±0.0001)	0.4651
Mass of wire before combustion(gr) (±0.0001)	0.0227
Mass of wire after combustion(gr) (±0.0001)	0.0167
Percentage of moist	%1.0
Percentage of ash	%7.1
Percentage of H	%5.24
Percentage of S	%0.5
Percentage of C	%88.29
Percentage of N	%1.01
Percentage of O	%4.96

Table 1: the masses of materials and percentages of elements present in the Zonguldak coal used throughout the experiment

Time (min)	Temperature of system in 1st Phase (°C) (±0.001)	ΔT (°C) $(T_{n+1} - T_n)$	Temperature of system in 2nd Phase (°C) (±0.001)	Temperature of system in 3rd Phase (°C) (±0.001)	ΔT (°C) $(T_{n+1} - T_n)$
1	18.290	0.000	18.600	19.375	0.000
2	18.290	0.010	19.080	19.375	0.005
3	18.280	0.000	19.260	19.370	0.005
4	18.280	0.005	19.325	19.365	0.005
5	18.275	0.045	19.365	19.360	0.000
6	18.320	0.000	19.375	19.360	0.005
7	18.320	0.005	19.375	19.355	0.005
8	18.315	0.005	19.375	19.350	0.005
9	18.310	0.000	19.375	19.340	0.000
10	18.310	0.000	-	19.340	0.005
11	18.310	0.010	-	19.335	0.005
12	18.300	0.000	-	19.330	0.005
13	18.300	-	-	19.325	0.005
14	18.300	-	-	19.320	0.000
15	18.300	-	-	19.320	0.010
16	18.300	-	-	19.310	0.000
17	-	-	-	19.310	0.005
18	-	-	-	19.305	0.005
19	-	-	-	19.300	0.005
20	-	-	-	19.295	0.005
21	-	-	-	19.295	-

Table 2: the changes of temperature in the 1st, 2nd and 3rd phases of the combustion reaction in the experiment

Graph 1: the change in temperature vs time in the combustion reaction of Zonguldak coal
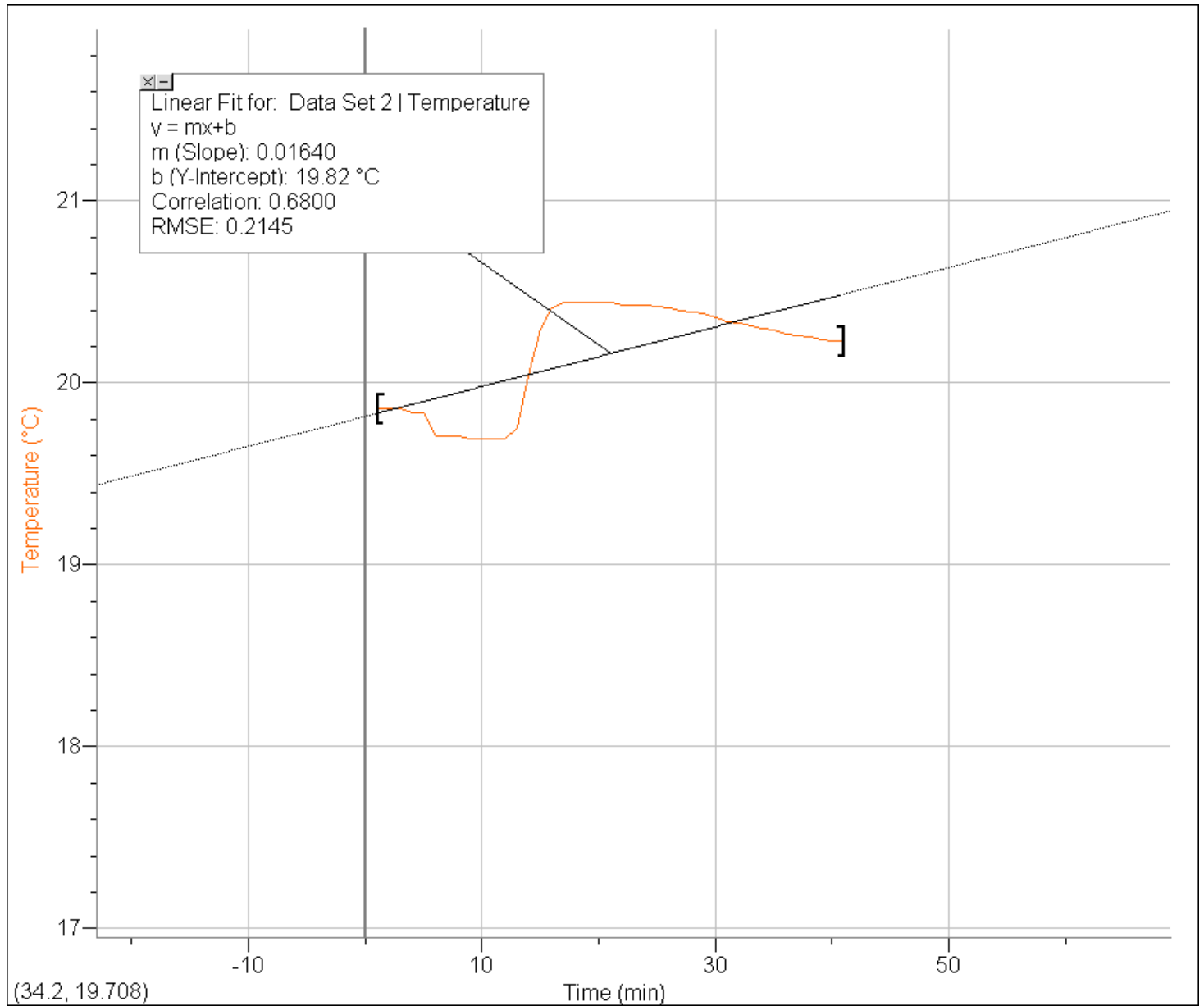
EXPERIMENT B – Subbituminous (Beypazarı coal)

Mass of sample with wire (gr) (±0.0001)	0.8567
Mass of wire before combustion(gr) (±0.0001)	0.0240
Mass of wire after combustion(gr) (±0.0001)	0.0112
Percentage of moist	%13.0
Percentage of ash	%37.77
Percentage of H	%5.29
Percentage of S	%9.14
Percentage of C	%62.50
Percentage of N	%2.07
Percentage of O	%21.00

Table 3: the masses of materials and percentages of elements present in the Beypazarı coal used throughout the experiment

Time (min)	Temperature of system in 1st Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1} - T_n\right)$	Temperature of system in 2nd Phase (°C) (±0.001)	Temperature of system in 3rd Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1} - T_n\right)$
1	19.860	0.000	19.690	20.430	0.010
2	19.860	0.000	19.750	20.420	0.010
3	19.860	0.020	20.040	20.410	0.010
4	19.840	0.000	20.300	20.400	0.010
5	19.840	0.130	20.410	20.390	0.010
6	19.710	0.000	20.440	20.380	0.020
7	19.710	0.000	20.440	20.360	0.020
8	19.710	0.020	20.440	20.340	0.010
9	19.690	0.000	20.440	20.330	0.020
10	19.690	0.000	20.440	20.310	0.010
11	19.690	-	20.430	20.300	0.010
12	-	-	20.430	20.290	0.020
13	-	-	-	20.270	0.010
14	-	-	-	20.260	0.010
15	-	-	-	20.250	0.010
16	-	-	-	20.240	0.010
17	-	-	-	20.230	0.000
18	-	-	-	20.230	-
19	-	-	-	-	-
20	-	-	-	-	-
21	-	-	-	-	-

Table 4: the changes of temperature in the 1st, 2nd and 3rd phases of the combustion reaction in the experiment

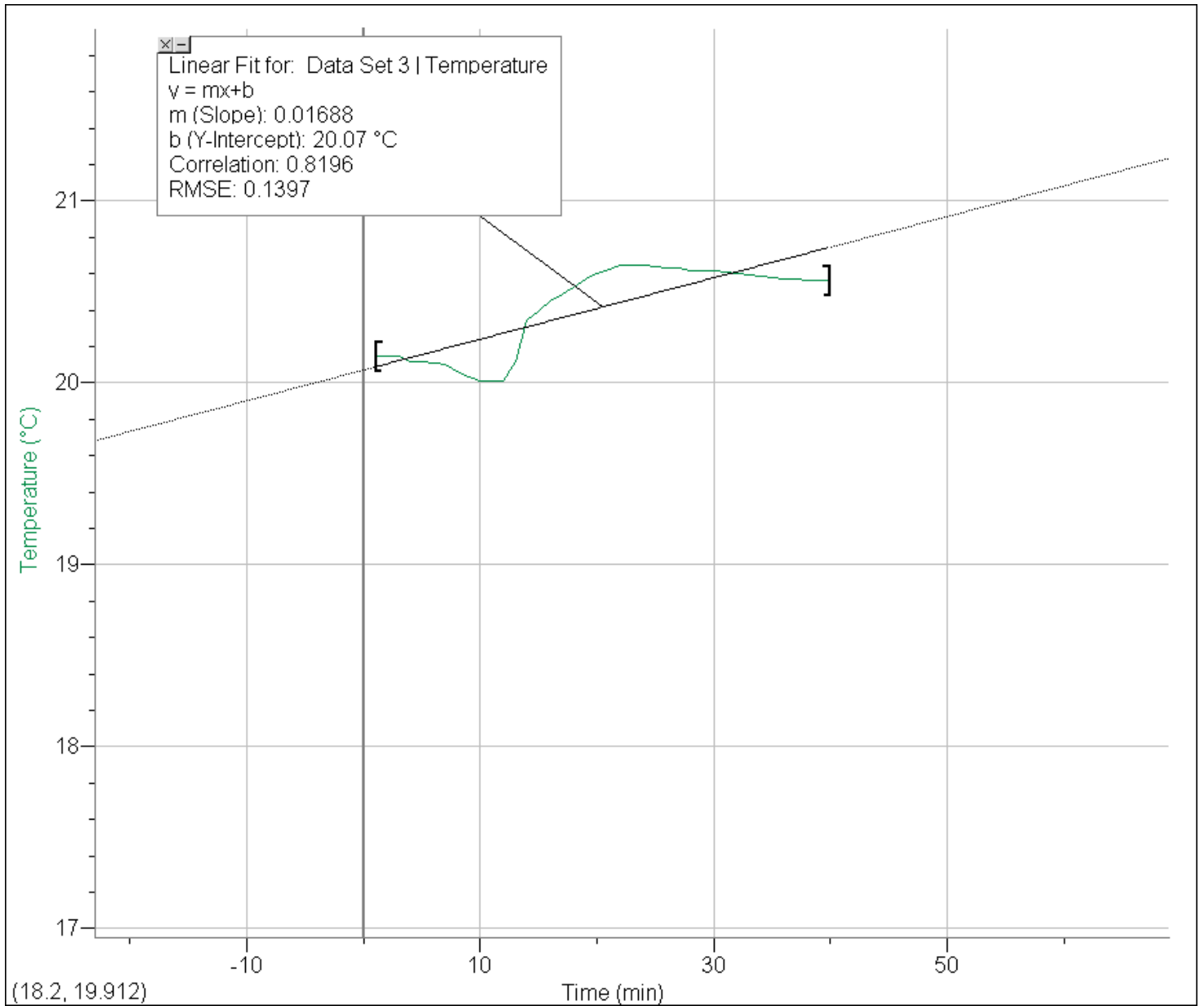Graph 2: the change in temperature vs time in the combustion reaction of Beypazarı coal

EXPERIMENT C – Lignite (Soma coal)

Mass of sample with wire (gr) (±0.0001)	0.8356
Mass of wire before combustion(gr) (±0.0001)	0.0190
Mass of wire after combustion(gr) (±0.0001)	0.0089
Percentage of moist	%22.69
Percentage of ash	%10.26
Percentage of H	%6.15
Percentage of S	%8.30
Percentage of C	%33.25
Percentage of N	%3.08
Percentage of O	%16.00

Table 5: the masses of materials and percentages of elements present in the Soma coal used throughout the experiment

Time (min)	Temperature of system in 1st Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1}-T_n\right)$	Temperature of system in 2nd Phase (°C) (±0.001)	Temperature of system in 3rd Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1}-T_n\right)$
1	20.150	0.000	20.013	20.650	0.010
2	20.150	0.000	20.113	20.640	0.005
3	20.150	0.030	20.345	20.635	0.005
4	20.120	0.005	20.395	20.630	0.010
5	20.115	0.005	20.447	20.620	0.000
6	20.110	0.005	20.485	20.620	0.005
7	20.105	0.038	20.525	20.615	0.005
8	20.067	0.020	20.575	20.610	0.005
9	20.035	0.032	20.605	20.605	0.010
10	20.013	0.000	20.625	20.595	0.010
11	20.013	-	20.650	20.585	0.005
12	-	-	20.650	20.580	0.010
13	-	-	-	20.570	0.000
14	-	-	-	20.570	0.005
15	-	-	-	20.565	0.000
16	-	-	-	20.565	-
17	-	-	-	20.565	-
18	-	-	-	-	-
19	-	-	-	-	-
20	-	-	-	-	-
21	-	-	-	-	-

Table 6: the changes of temperature in the 1st, 2nd and 3rd phases of the combustion reaction in the experiment

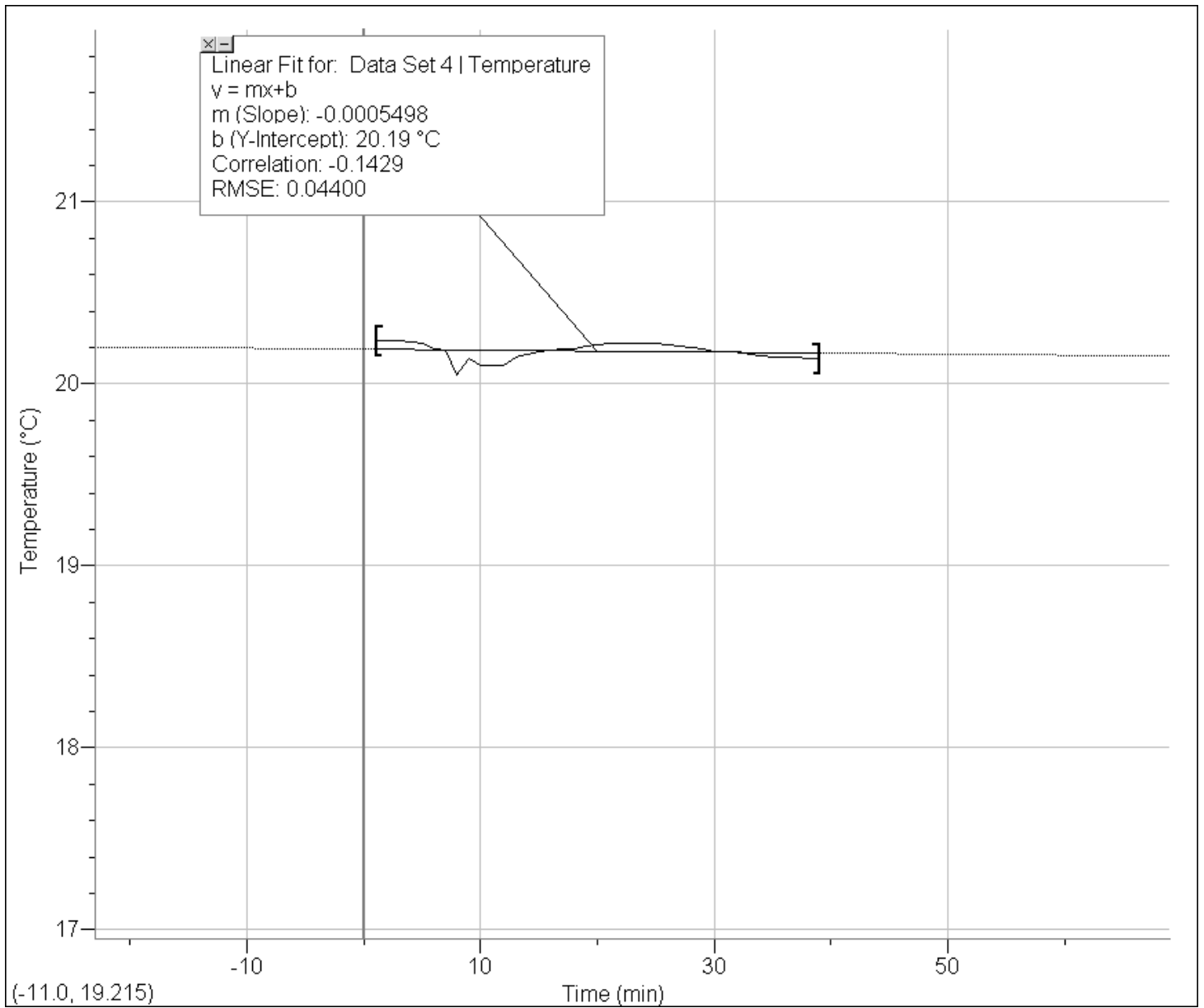Graph 3: the change in temperature vs time in the combustion reaction of Soma coal

EXPERIMENT D - Octane

Mass of sample (gr) (±0.0001)	0.4356
Mass of wire before combustion(gr) (±0.0001)	0.0203
Mass of wire after combustion(gr) (±0.0001)	0.0153
Percentage of moist	-
Percentage of ash	-
Percentage of H	%15.78
Percentage of S	-
Percentage of C	%84.21
Percentage of N	-
Percentage of O	-

Table 7: the masses of materials and percentages of elements present in the octane used throughout the experiment

Time (min)	Temperature of system in 1st Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1} - T_n\right)$	Temperature of system in 2nd Phase (°C) (±0.001)	Temperature of system in 3rd Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1} - T_n\right)$
1	20.235	0.000	20.105	20.225	0.005
2	20.235	0.000	20.145	20.220	0.005
3	20.235	0.005	20.165	20.215	0.005
4	20.230	0.005	20.175	20.210	0.010
5	20.225	0.030	20.185	20.200	0.010
6	20.195	0.010	20.190	20.190	0.010
7	20.185	0.038	20.190	20.180	0.005
8	20.047	0.010	20.210	20.175	0.000
9	20.137	0.032	20.215	20.175	0.010
10	20.105	0.000	20.220	20.165	0.010
11	20.105	-	20.225	20.155	0.005
12	-	-	20.225	20.150	0.000
13	-	-	-	20.150	0.005
14	-	-	-	20.145	0.005
15	-	-	-	20.140	0.000
16	-	-	-	20.140	-
17	-	-	-	-	-
18	-	-	-	-	-
19	-	-	-	-	-
20	-	-	-	-	-
21	-	-	-	-	-

Table 8: the changes of temperature in the 1st, 2nd and 3rd phases of the combustion reaction in the experiment

Graph 4: the change in temperature vs time in the combustion reaction of octane
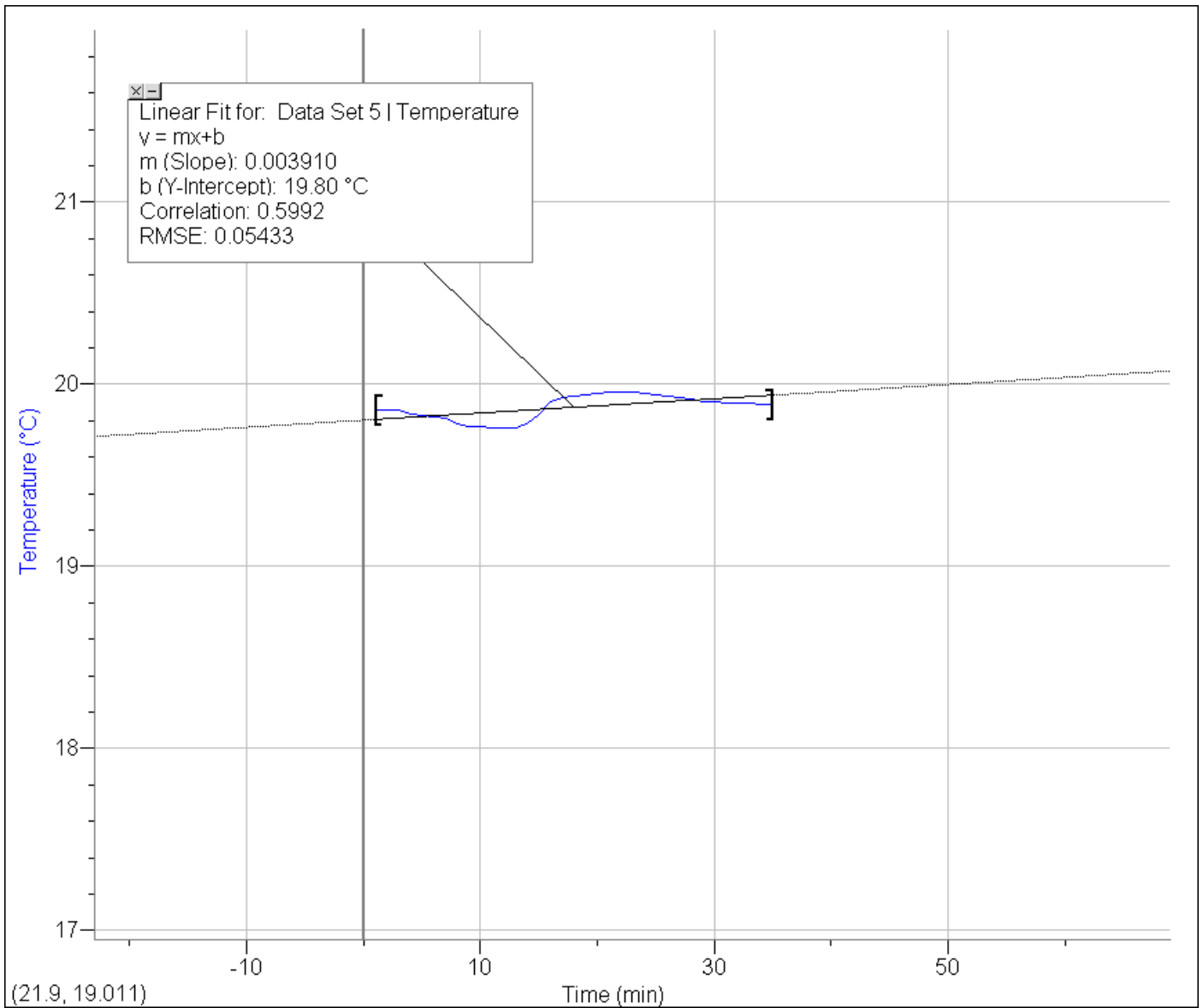
EXPERIMENT E – Dodecane

Mass of sample (gr) ($\pm$0.0001)	0.4135
Mass of wire before combustion(gr) ($\pm$0.0001)	0.0195
Mass of wire after combustion(gr) ($\pm$0.0001)	0.0087
Percentage of moist	-
Percentage of ash	-
Percentage of H	%15.30
Percentage of S	-
Percentage of C	%84.70
Percentage of N	-
Percentage of O	-

Table 9: the masses of materials and percentages of elements present in the dodecane used throughout the experiment

Time (min)	Temperature of system in 1st Phase (°C) ($\pm$0.001)	ΔT (°C) $\left(T_{n+1} - T_n\right)$	Temperature of system in 2nd Phase (°C) ($\pm$0.001)	Temperature of system in 3rd Phase (°C) ($\pm$0.001)	ΔT (°C) $\left(T_{n+1} - T_n\right)$
1	19.860	0.000	19.760	19.956	0.005
2	19.860	0.000	19.785	19.951	0.005
3	19.860	0.030	19.835	19.946	0.010
4	19.835	0.005	19.905	19.936	0.010
5	19.830	0.005	19.925	19.926	0.005
6	19.825	0.010	19.935	19.921	0.015
7	19.815	0.035	19.943	19.906	0.005
8	19.780	0.010	19.953	19.901	0.005
9	19.770	0.005	19.956	19.896	0.000
10	10.765	0.005	19.956	19.896	0.000
11	19.760	0.000	-	19.896	0.005
12	19.760	-	-	19.891	0.000
13	-	-	-	19.891	-
14	-	-	-	-	-
15	-	-	-	-	-
16	-	-	-		-
17	-	-	-	-	-
18	-	-	-	-	-
19	-	-	-	-	-
20	-	-	-	-	-
21	-	-	-	-	-

Table 10: the changes of temperature in the 1st, 2nd and 3rd phases of the combustion reaction in the experiment

Graph 5: the change in temperature vs time in the combustion reaction of dodecane

EXPERIMENT F – Hexadecane

Mass of sample (gr) (±0.0001)	0.4605
Mass of wire before combustion(gr) (±0.0001)	0.0201
Mass of wire after combustion(gr) (±0.0001)	0.0094
Percentage of moist	-
Percentage of ash	-
Percentage of H	%15.05
Percentage of S	-
Percentage of C	%84.95
Percentage of N	-
Percentage of O	-

Table 11: the masses of materials and percentages of elements present in the hexadecane used throughout the experiment

Time (min)	Temperature of system in 1st Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1}-T_n\right)$	Temperature of system in 2nd Phase (°C) (±0.001)	Temperature of system in 3rd Phase (°C) (±0.001)	ΔT (°C) $\left(T_{n+1}-T_n\right)$
1	19.922	0.000	19.856	20.216	0.005
2	19.922	0.000	19.876	20.211	0.010
3	19.922	0.005	19.911	20.201	0.010
4	19.917	0.005	19.962	20.191	0.010
5	19.912	0.005	20.064	20.181	0.005
6	19.907	0.010	20.113	20.176	0.005
7	19.897	0.010	20.175	20.171	0.005
8	19.887	0.010	20.195	20.166	0.000
9	19.877	0.010	20.205	20.166	0.010
10	19.867	0.005	20.210	20.156	0.010
11	19.861	0.005	20.216	20.146	0.005
12	19.856	0.000	20.216	20.141	0.000
13	19.856	-	-	20.141	0.005
14	-	-	-	20.136	0.005
15	-	-	-	20.131	0.005
16	-	-	-	20.126	0.005
17	-	-	-	-	0.000
18	-	-	-	-	-
19	-	-	-	-	-
20	-	-	-	-	-
21	-	-	-	-	-

Table 12: the changes of temperature in the 1st, 2nd and 3rd phases of the combustion reaction in the experiment
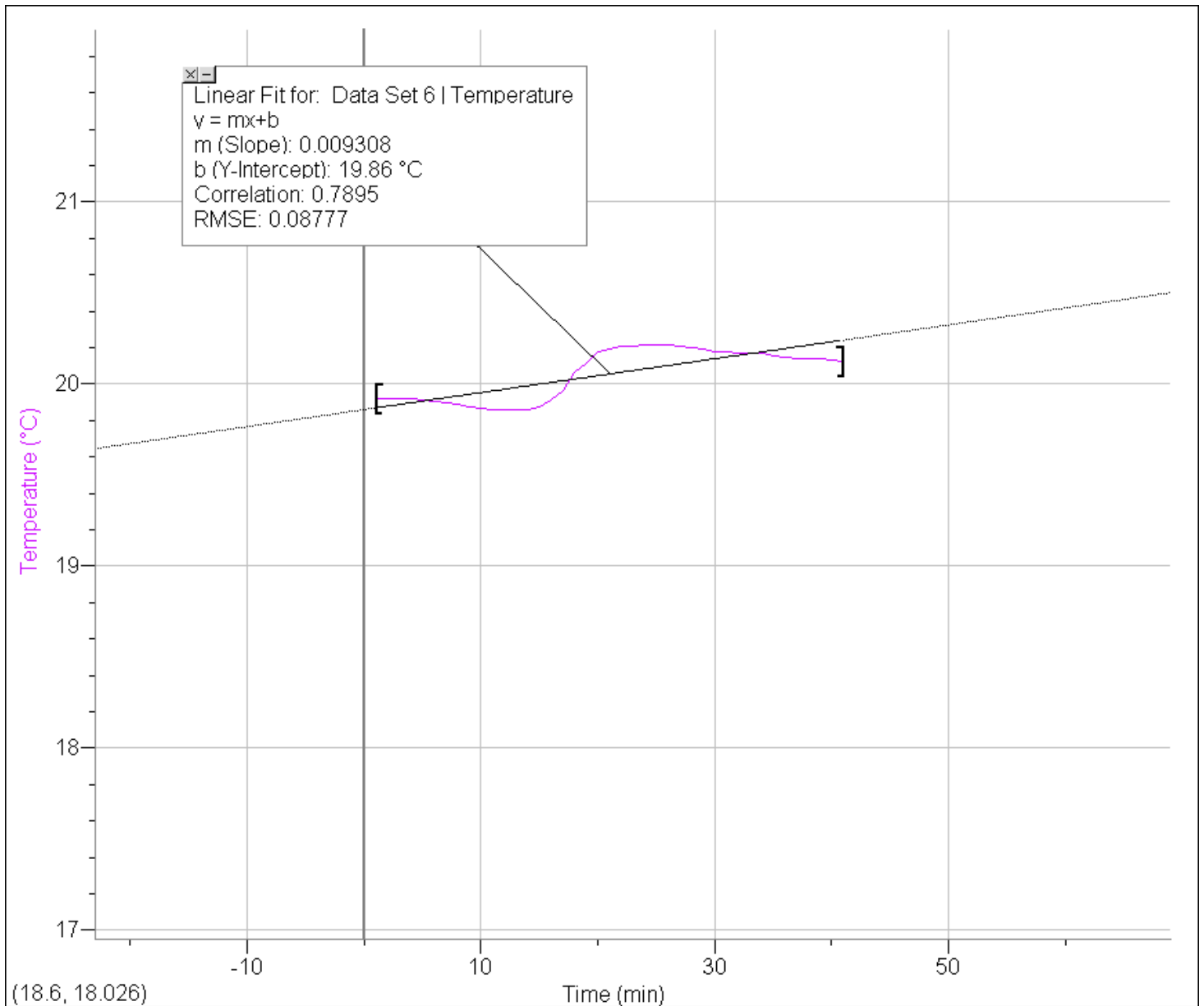
Graph 6: the change in temperature vs time in the combustion reaction of hexadecane

DATA ANALYSIS

Calculation of Higher/Lower Heating values and Amounts of Air Pollutans released from Bituminous coal (Zonguldak Coal)

Higher Heating Value

t_m : 19.375 C
m : 10
t_0 : 18.30 C

$v = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{12}) / 12 = 0.0067$

$n = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{20}) / 20 = 0.004$

F = 1.0 because $\Delta T_1 = 0.48$ and $\Delta T_2 = 0.18$ so $\Delta T_1 > \Delta T_2$

$$c = n\,x\,m - (n + v)\,x\,F$$

$$c = 0.004\,x\,10 - (0.004 + 0.0067)\,x\,1.0 = 0.0293$$

As there is really small amounts of S and N in the sample while calculating b value these are neglected.

Burnt wire = 0.0227 – 0.0167 = 0.006 g = 6 mg

$$b = bD = 6mg\,x\,1.6\,\frac{cal}{mg} = 9.6\,cal$$

msample = 0.4651 – 0.0227 = 0.4424 g

$$G = msample = 0.4424 - 0.4424\,x\,(0.071 + 0.01) = 0.4066\,g$$

$$H_0 = \frac{W\,x\,(t_m + c - t_0) - b}{G}$$

$$H_0 = \frac{3300\,x\,(19.375 + 0.0293 - 18.30) - 9.6}{0.4066} = 8939.7\,\frac{cal}{g}$$

Lower Heating Value

$$H_u = H_0 - 5.85 \, x \, (9H + K)$$

$$H_u = 8939.7 - 5.85 \, x \, (9 \, x \, 5.24 + 1.0) = 8657.57 \, \frac{cal}{g}$$

Amount of CO_2, N_2O_5, SO_3 released from the reaction

Amount of C : $\dfrac{\dfrac{88.29}{100} \, x \, 0.4424g}{12 \left(\dfrac{g}{mol} \right)} = 0.033 \, mol$

$C_s \quad + \quad O_{2(g)} \rightarrow CO_{2(g)}$
0.033 mol $\qquad\qquad$ 0.033 mol CO_2 released from 0.4424g Zonguldak Coal
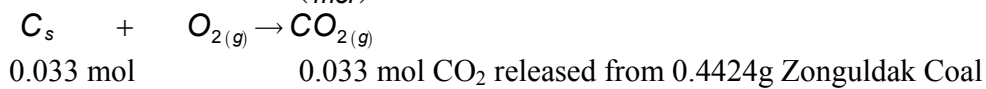
$\dfrac{0.033}{0.4424} = 0.075 \, mol$ CO_2 released from 1g Zonguldak Coal

Amount of N : $\dfrac{\dfrac{1.01}{100} \, x \, 0.4424g}{14 \left(\dfrac{g}{mol} \right)} = 3.19 \, x10^{-4} \, mol$

$4N_{(s)} \quad + \quad 5O_{2(g)} \rightarrow 2N_2O_{5(g)}$
3.19 x 10⁻⁴ $\qquad\qquad$ 1.59 x 10⁻⁴ mol N_2O_5 released from 0.4424g Zonguldak Coal
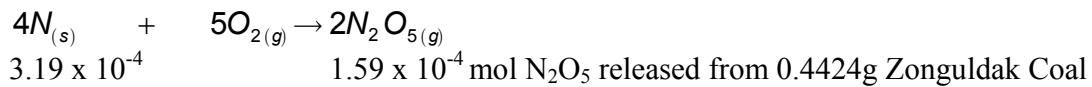
$\dfrac{1.59 \, x10^{-4}}{0.4424} = 3.61 \, x10^{-4} \, mol$ N_2O_5 released from 1g Zonguldak Coal

Amount of S : $\dfrac{\dfrac{0.5}{100} \, x \, 0.4424g}{32.07 \left(\dfrac{g}{mol} \right)} = 6.89 \, x10^{-5} \, mol$

$2S_{(s)} \quad + \quad 3O_{2(g)} \rightarrow 2SO_{3(g)}$
6.89 x 10⁻⁵ $\qquad\qquad$ 6.89 x 10⁻⁵ mol SO_3 released from 0.4424g Zonguldak Coal
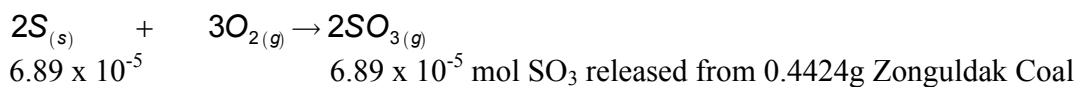
$\dfrac{6.89 \, x10^{-5}}{0.4424} = 1.56 \, x10^{-4} \, mol$ SO_3 released from 1g Zonguldak Coal

Alican Salor
001129–057

Calculation of Higher/Lower Heating values and Amounts of Air Pollutans released from Subbituminous coal(Beypazarı coal)

t_m : 20.43 C
m : 12
t_0 : 19.69 C

$v = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{10}) / 10 = 0.017$

$n = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{17}) / 17 = 0.012$

F = 1.5 because $\Delta T_1 = 0.06$ and $\Delta T_2 = 0.29$ so $\Delta T_2 > \Delta T_1$

$$c = n \, x \, m - (n + v) \, x \, F$$

$$c = 0.012 \, x \, 12 - (0.012 + 0.017) \, x 1.5 = 0.1005$$

As there is really small amounts of S and N in the sample while calculating b value these are neglected.

Burnt wire = 0.0240 – 0.0112 = 0.0128 g = 12.8 mg

$$b = bD = 12mg \, x \, 1.6 \, \frac{cal}{mg} = 19.2 \, cal$$

msample = 0.8567 – 0.0240 = 0.8327 g

$$G = msample = 0.8327 - 0.8327 \, x \, (0.37 + 0.13) = 0.4080 \, g$$

$$H_0 = \frac{W \, x \left(t_m + c - t_0\right) - b}{G}$$

$$H_0 = \frac{3300 \, x \, (20.43 + 0.1005 - 19.69) - 19.2}{0.4080} = 6751.10 \, \frac{cal}{g}$$

Lower Heating Value

$$H_u = H_0 - 5.85 \, x \, (9H + K)$$

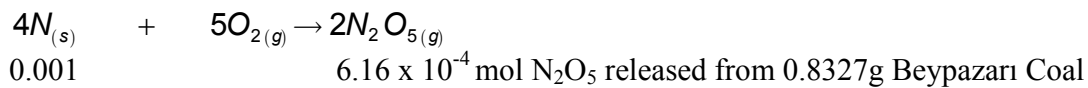$$H_u = 6751.10 - 5.85 \, x \, (9 \, x \, 5.29 + 13.0) = 6396.53 \, \frac{cal}{g}$$

Alican Salor
001129–057

Amount of CO₂, N₂O₅, SO₃ released from the reaction

Amount of C : $\dfrac{\dfrac{62.50}{100} \times 0.8327g}{12\left(\dfrac{g}{mol}\right)} = 0.043\ mol$

$C_s\quad +\quad O_{2(g)} \rightarrow CO_{2(g)}$
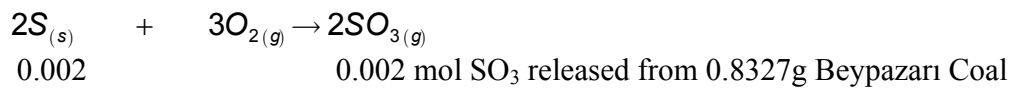
0.043   0.043 mol CO₂ released from 0.8327g Beypazarı Coal
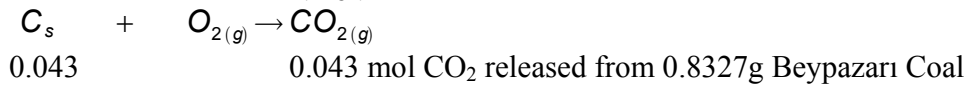
$\dfrac{0.043}{0.8327} = 0.051\ mol$ CO₂ released from 1g Beypazarı Coal

Amount of N : $\dfrac{\dfrac{2.07}{100} \times 0.8327g}{14\left(\dfrac{g}{mol}\right)} = 0.001\ mol$

$4N_{(s)}\quad +\quad 5O_{2(g)} \rightarrow 2N_2O_{5(g)}$

0.001   6.16 x 10⁻⁴ mol N₂O₅ released from 0.8327g Beypazarı Coal

$\dfrac{6.16 \times 10^{-4}}{0.8327} = 7.39 \times 10^{-4}\ mol$ N₂O₅ released from 1g Beypazarı Coal

Amount of S : $\dfrac{\dfrac{9.14}{100} \times 0.8327g}{32.07\left(\dfrac{g}{mol}\right)} = 0.002\ mol$

$2S_{(s)}\quad +\quad 3O_{2(g)} \rightarrow 2SO_{3(g)}$

0.002   0.002 mol SO₃ released from 0.8327g Beypazarı Coal

$\dfrac{0.001}{0.8327} = 0.0012\ mol$ SO₃ released from 1g Beypazarı Coal

Calculation of Higher/Lower Heating values and Amounts of Air Pollutans released from Lignite (Soma coal)

t_m : 20.650 C
m : 12
t_0 : 20.013 C

$v = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{10}) / 10 = 0.014$

n = (ΔT$_1$ + ΔT$_2$ + ΔT$_3$ + ... + ΔT$_{17}$) / 17 = 0.006

F = 1.5 because ΔT$_1$ = 0.1 and ΔT$_2$ = 0.232 so ΔT$_2$ > ΔT$_1$

$$c = n \times m - (n + v) \times F$$

$$c = 0.006 \times 12 - (0.006 + 0.014) \times 1.5 = 0.042$$

As there is really small amounts of S and N in the sample while calculating b value these are neglected.

Burnt wire = 0.0190 – 0.0089 = 0.0101 g = 10.1mg

$$b = bD = 10.1mg \times 1.6 \frac{cal}{mg} = 16.6\ cal$$

msample = 0.8356 – 0.0190 = 0.8166 g

$$G = msample = 0.8166 - 0.8166 \times (0.23 + 0.11) = 0.5389\ g$$

$$H_0 = \frac{W \times (t_m + c - t_0) - b}{G}$$

$$H_0 = \frac{3300 \times (20.650 + 0.042 - 20.013) - 16.6}{0.5389} = 4127.11 \frac{cal}{g}$$

Lower Heating Value
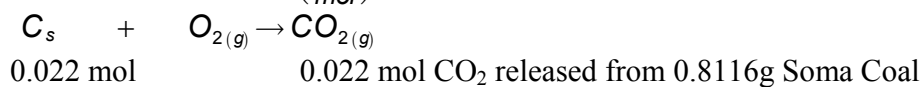
$$H_u = H_0 - 5.85 \times (9H + K)$$

$$H_u = 4127.11 - 5.85 \times (9 \times 6.15 + 22.69) = 3670.57 \frac{cal}{g}$$

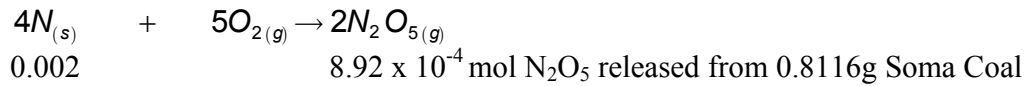**Amount of CO$_2$, N$_2$O$_5$, SO$_3$ released from the reaction**

Amount of C : $\dfrac{\dfrac{33.25}{100} \times 0.8116g}{12 \left(\dfrac{g}{mol} \right)} = 0.022\ mol$

$$C_s\ \ +\ \ O_{2(g)} \to CO_{2(g)}$$

0.022 mol $\qquad\qquad$ 0.022 mol CO$_2$ released from 0.8116g Soma Coal

$$\frac{0.022}{0.8116} = 0.027\ mol\ \text{CO}_2\ \text{released from 1g Soma Coal}$$

Amount of N : $\dfrac{\dfrac{3.08}{100}\,x\,0.8116g}{14\left(\dfrac{g}{mol}\right)} = 0.002\ mol$

$4N_{(s)}\quad +\quad 5O_{2\,(g)} \rightarrow 2N_2O_{5\,(g)}$
0.002 $\qquad\qquad$ 8.92 x 10^{-4} mol N_2O_5 released from 0.8116g Soma Coal

$$\frac{8.92\,x10^{-4}}{0.8116} = 0.0011\ mol\ \text{N}_2\text{O}_5\ \text{released from 1g Soma Coal}$$

Amount of S : $\dfrac{\dfrac{8.30}{100}\,x\,0.8116g}{32.07\left(\dfrac{g}{mol}\right)} = 0.002\ mol$

$2S_{(s)}\quad +\quad 3O_{2\,(g)} \rightarrow 2SO_{3\,(g)}$
0.002 $\qquad\qquad$ 0.002 mol SO_3 released from 0.8116g Soma Coal

$$\frac{0.002}{0.4424} = 0.0024\ mol\ \text{SO}_3\ \text{released from 1g Soma Coal}$$

Calculation of Higher/Lower Heating values and Amounts of Air Pollutans released from Octane

t_m : 20.225 C
m : 12
t_0 : 20.105 C

$v = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{10}) / 10 = 0.013$

$n = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{16}) / 16 = 0.005$

F = 1.0 because $\Delta T_1 = 0.04$ and $\Delta T_2 = 0.02$ so $\Delta T_1 > \Delta T_2$

$c = n\,x\,m - (n + v)\,x\,F$

$c = 0.005\,x\,12 - (0.005 + 0.013)\,x1.0 = 0.042$

Burnt wire = 0.0203 – 0.0153 = 0.005 g = 5mg

$$b = bD = 5mg \ x \ 1.6 \ \frac{cal}{mg} = 8 \ cal$$

$G = 0.4356$ g

$$H_0 = \frac{W \ x \ (t_m + c - t_0) - b}{G}$$

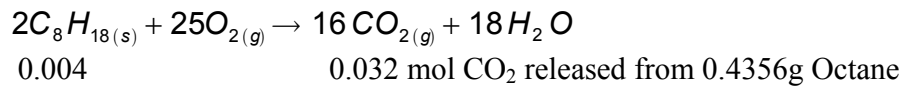$$H_0 = \frac{3300 \ x \ (20.225 + 0.042 - 20.105) - 8}{0.4356} = 1208.90 \ \frac{cal}{g}$$

Lower Heating Value

$$H_u = H_0 - 5.85 \ x \ (9H + K)$$

$$H_u = 1208.90 - 5.85 \ x \ 15.78 = 1116.587 \ \frac{cal}{g}$$

Amount of CO_2 released from the reaction

Amount of C_8H_{18} : $\dfrac{0.4356g}{114 \ \frac{g}{mol}} = 0.004 \ mol$

$$2C_8H_{18 \, (s)} + 25O_{2 \, (g)} \rightarrow 16 \, CO_{2 \, (g)} + 18 \, H_2O$$

 0.004   0.032 mol CO_2 released from 0.4356g Octane

$\dfrac{0.032}{0.4356} = 0.0701 \ mol$ CO_2 released from 1g Octane

Calculation of Higher/Lower Heating values and Amounts of Air Pollutans released from Dodecane

t_m : 19.956 C
m : 10
t_0 : 19.760 C

$v = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{11}) / 11 = 0.009$

$n = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{12}) / 12 = 0.005$

$F = 1.0$ because $\Delta T_1 = 0.025$ and $\Delta T_2 = 0.05$ so $\Delta T_1 > \Delta T_2$

$$c = n \, x \, m - (n + v) \, x \, F$$

$$c = 0.005 \, x \, 10 - (0.005 + 0.013) \, x \, 1.0 = 0.036$$

Burnt wire $= 0.0195 - 0.0087 = 0.0108 \, g = 10.8 mg$

$$b = bD = \; 10.8 mg \, x \, 1.6 \, \frac{cal}{mg} = 17.28 \, cal$$

$G = 0.4135 \, g$

$$H_0 = \frac{W \, x \, (t_m + c - t_0) - b}{G}$$

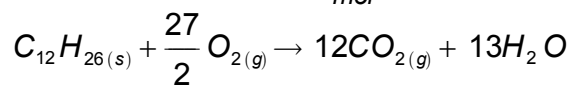$$H_0 = \frac{3300 \, x \, (19.956 + 0.036 - 19.760) - 17.28}{0.4135} = 1809.72 \, \frac{cal}{g}$$

Lower Heating Value

$$H_u = H_0 - 5.85 \, x \, (9H + K)$$
$$H_u = 1809.72 - 5.85 \, x \, 15.30 = 1720.215 \, \frac{cal}{g}$$

Amount of CO$_2$ released from the reaction

Amount of $C_{12}H_{26}$: $\;\dfrac{0.4135 g}{170 \, \frac{g}{mol}} = 0.0024 \, mol$

$$C_{12}H_{26\,(s)} + \frac{27}{2} O_{2\,(g)} \rightarrow 12 CO_{2\,(g)} + 13 H_2 O$$

0.0024   0.029 mol CO$_2$ released from 0.4135g Dodecane

$\dfrac{0.029}{0.4135} = 0.0705 \, mol$ CO$_2$ released from 1g Dodecane

Calculation of Higher/Lower Heating values and Amounts of Air Pollutans released from Hexadecane

t_m : 20.216 C
m : 12
t_0 : 19.856 C

30

$v = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{12}) / 12 = 0.005$

$n = (\Delta T_1 + \Delta T_2 + \Delta T_3 + \ldots + \Delta T_{17}) / 17 = 0.006$

F = 1.5 because $\Delta T_1 = 0.02$ and $\Delta T_2 = 0.035$ so $\Delta T_1 > \Delta T_2$

$$c = n \, x \, m - (n + v) \, x \, F$$

$$c = 0.006 \, x \, 12 - (0.006 + 0.005) \, x 1.5 = 0.06$$

Burnt wire = $0.0201 - 0.0094 = 0.0108$ g = 10.7mg

$$b = bD = \; 10.7 mg \, x \, 1.6 \, \frac{cal}{mg} = 17.12 \, cal$$

G = 0.4605 g

$$H_0 = \frac{W \, x \, (t_m + c - t_0) - b}{G}$$

$$H_0 = \frac{3300 \, x \, (20.216 + 0.06 - 19.856) - 17.12}{0.4605} = 2972.56 \, \frac{cal}{g}$$
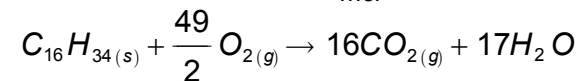
Lower Heating Value

$$H_u = H_0 - 5.85 \, x \, (9H + K)$$
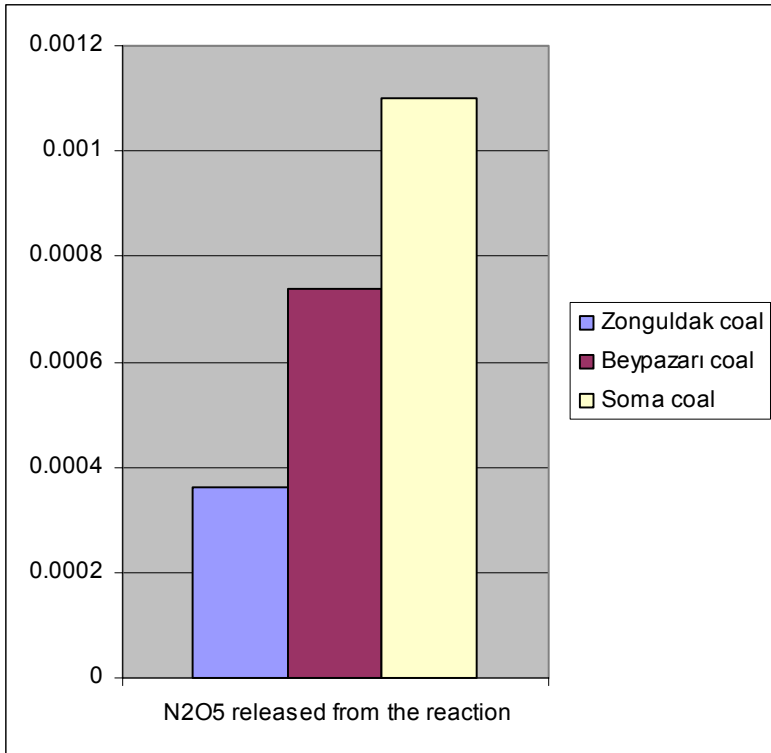
$$H_u = 2972.56 - 5.85 \, x \, 15.05 = 2884.51$$

Amount of CO$_2$ released from the reaction

Amount of $C_{16}H_{34}$: $\dfrac{0.4605g}{226 \, \frac{g}{mol}} = 0.002 \, mol$

$$C_{16}H_{34\,(s)} + \frac{49}{2} O_{2\,(g)} \rightarrow 16CO_{2\,(g)} + 17H_2O$$

0.002   0.033 mol CO$_2$ released from 0.4605g Hexadecane

$$\frac{0.033}{0.4605} = 0.0707 \, mol \; \text{CO}_2 \text{ released from 1g Hexadecane}$$

Alican Salor
001129–057

Graph 7: amount of N_2O_5 released from the combustion reactions of Zonguldak, Beypazarı, Soma coals
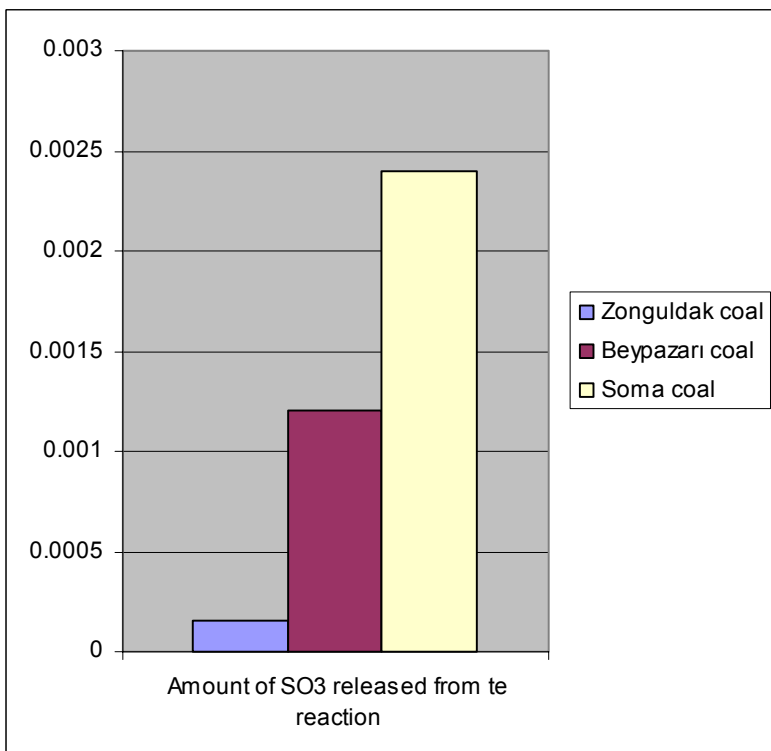
Graph 8: amount of SO_3 released from the combustion reactions of Zonguldak, Beypazarı, Soma coals

Alican Salor
001129–057
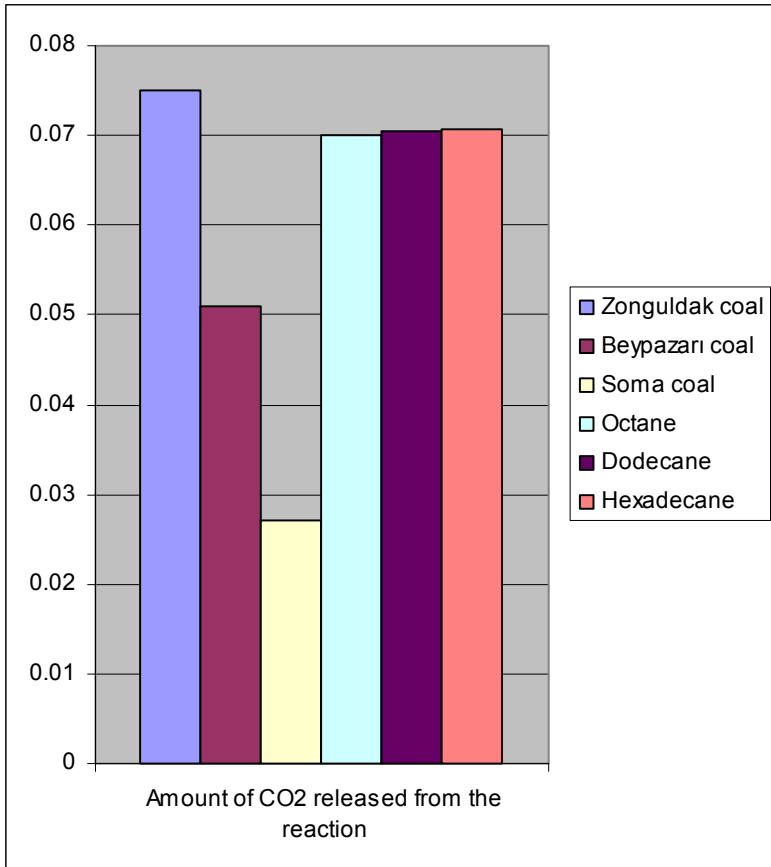
Graph 9: amount of CO_2 released from the combustion reactions of Zonguldak, Beypazarı, Soma coals, octane, dodecane and hexadecane
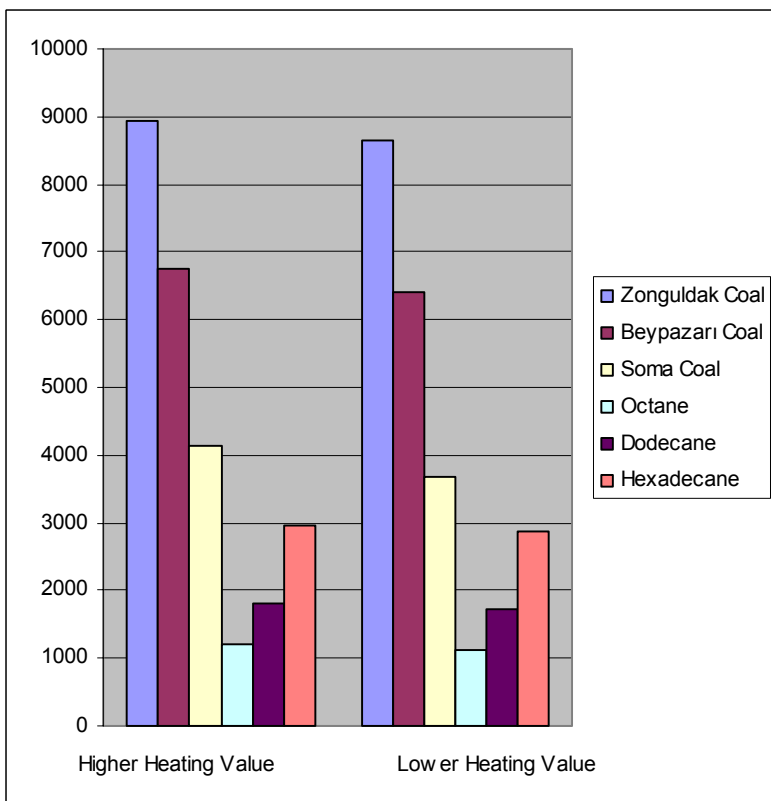
Graph 10: the lower and higher heating values of the combustion reactions of Zonguldak, Beypazarı, Soma coals, octane, dodecane and hexadecane

Conclusion And Evaluation

In this extended essay the efficiency and the damage cause to the environment by the release of CO_2 and other harmful gases of the widely used carbon based fuels ,such as coal and petroleum, are compared.

In this project Zonguldak coal (a bituminous coal sample), Beypazarı coal (a subbituminous coal sample) and Soma coal(a lignite sample) is used as widely used coals. Because antrachite is hard to find and has an expensive price, this coal type is not used. On the other hand no petroleum is used in this project however, in order to get close heat values, hydrocarbons that have high usage percentage in different types of petroleum are used. For example, octane (present in gasoline), dodecane (present in diesel fuel) and hexadecane (found in kerosene). Moreover a bomb calorimeter is used to determine the heat values of the fuels. Other calculations that include the amount of CO_2, SO_3, N_2O_5 released from the reactions are theoretical values. The amounts of SO_3 and N_2O_5 could only be found when using coal types because hydrocarbons that where used in the experiment doesn't contain any S or N elements. And because the combustion was done in a bomb calorimeter (a closed system) using pure O_2, air that contains S, N wasn't involved in the reactions.

Another important thing that must be know about the project is that because all the experiments where made room conditions and in a bomb calorimeter which is a closed system the water formed from the combustion reaction condenses so, the value found is the higher heating value. However lower heating value can be found too because the difference between these values is the latent heat of evaporization.

First of all, the higher and lower heating values of Zonguldak coal are found to be respectively 8939.7 cal/g and 8657.57 cal/g. From the graph 1 it can be seen that there is a great change in the temperature between 10-30th minutes. The phases before and after the great increase, the temperature tends to decrease. However this decrease can be neglected compared to the increase. Moreover the amounts of CO_2, SO_3 and N_2O_5 released from the reaction are found to be respectively 0.075mol/g, 1.56×10^{-4}mol/g, 3.61×10^{-4}mol/g.

Secondly the higher and lower heating values of Beypazarı coal are found to be respectively 6751.10 cal/g, 6396.53 cal/g. This is a little less than the heating values of Zonguldak coal. So the temperature change in the graph 2 is less too. The slope of this increase is about the same with Zonguldak coal. However the decrease of temperatures in the 1st and 3rd phases are more than Zonguldak coal. The amounts of CO_2, SO_3 and N_2O_5 released from the reaction are found to be respectively 0.051mol/g, 0.002mol/g and 7.39×10^{-4}mol/g.

The higher and lower heating values of Soma coal are respectively 4127.11 cal/g, 3670.57 cal/g. Among all the coal types this is the one with the least heating values. Moreover if the graph 3 is examined, it can be seen that the slope of 2nd phase is less than the other two coals types. More over this phase takes more time than the others as

the rate of the increase in temperature starts to decrease through the end of this phase. Apart from the heating values, the amounts of CO_2, SO_3 and N_2O_5 released from the reaction are respectively 0.027mol/g, 0.001mol/g, 0.0024mol/g.

If we take a look at Octane, the fuel with least heating value among all the fuels examined throughout the project, its higher heating value is found to be 1208.90 cal/g. From the graph it can be seen that the temperature increase in the second phase is really low and the decrease in the first phase is not orderly as the other fuel types. Moreover amount of CO2 released is 0.0701mol/g.

The other hydrocarbon type Dodecane, which is found in diesel fuels, has higher and lower heating values of respectively 1809.72cal/g and 1720.215cal/g. The change of temperature in second phase is still not much and the slope is not as vertical as seen in the coal types however the 1st and 3rd phases are more orderly than Octane. What's more the amount of CO2 released from the combustion reaction is 0.0705mol/g.

Lastly, with the higher and lower heating values of 2972.56cal/g and 2884.51cal/g Hexadecane is the hydrocarbon with the highest heating values among the hydrocarbons used in the experiment. From the graph 6 it can be seen that the slope temperature change in the second phase is much more vertical than the other hydrocarbons, and it is even close to thevalues found when using coal types. Moreover the CO_2 released from the reaction is found to be 0.0707mol/g.

From all these results it can be said that among all these different kinds of fuels Zonguldak coal which is a bituminous coal type has the greatest heating value. The comparison of heating values goes on like this (which can be seen from graph 10 too):
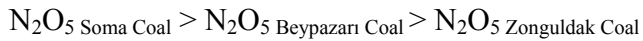
Heating Value $_{Zonguldak\ Coal}$ > Heating Value $_{Beypazarı\ Coal}$ > Heating Value $_{Soma\ Coal}$ >Heating Value $_{Hexadecane}$ > Heating Value $_{Dodecane}$ > Heating Value $_{Octane}$

Moreover it is seen from the comparison of the amount of CO_2 (graph 9) released among the fuel types which is:

CO_2 $_{Zonguldak\ Coal}$ > CO_2 $_{Beypazarı\ Coal}$ > CO_2 $_{Soma\ Coal}$ >CO_2 $_{Hexadecane}$ > CO_2 $_{Dodecane}$ > CO_2 $_{Octane}$

that as the heating value increases, the amount of CO_2 released from the combustion reaction into the atmosphere increase too. This is caused by the amount of C element present in each fuel that is used in the experiment. So this means that as the bond capacity of the fuel which is depedent on C element present is increased, the heat value will increase eventually, however at the same time increasing the amount of CO_2 into the environment. This plays a vital role in the efficiency of a carbon based fuel, because CO_2 is one of the primary air pollutants. It tends to allow incoming solar radiation to reach Earth but absorb some of the heat radiated from the Earth, increasing the greenhouse effect and thus increasing Earth's temperature So for the fuels to be efficient a balance between CO_2 and heating value must be reached.

Another comparison can be done between the amounts of N_2O_5 and SO_3 released into the atmosphere by these fuels (graph 7,8):

N_2O_5 Soma Coal $> N_2O_5$ Beypazarı Coal $> N_2O_5$ Zonguldak Coal

SO_3 Soma Coal $> SO_3$ Beypazarı Coal $> SO_3$ Zonguldak Coal

This comparison plays another vital role in determining the efficiency of these fuels too because N_2O_5 and SO_3 are much more dangerous air pollutants than CO_2. As these dissolve in H_2O present in the atmosphere they form:

$$SO_{3(g)} + H_2O_{(l)} \rightarrow H_2SO_{3(aq)}$$

$$N_2O_{5(g)} + H_2O_{(l)} \rightarrow 2HNO_{3(aq)}$$
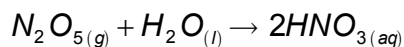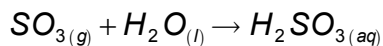
which are acidic solutions. So oxides of sulfur and nitrogen might not be greenhouse gases, but they cause acid rain (which is not just dangerous for human health however aquatic life and materials too),breathing problems and irritates the respiratory track.

Moreoever from this comparison it can be seen that amounts of SO_3 and N_2O_5 is effected by the amount of C element present in the fuel. As the C element present in the fuel increases, amounts of both N_2O_5 and SO_3 released into the atmosphere decrease. However ever still when amount of these gases decrease, CO_2 will increases. So these must be balanced.

On the other hand hydrocarbons used in the experiment doesn't even contain S or N which means that none of the oxides of nitrogen and sulfur will be produced when pure oxygen is used for the combustion.

With all these results concluded from this experiment, the comparison of efficiency of these fuels can be made in two different situations. In one of these situations we assume that all control methods of both SO_3 and N_2O_5 are present in the environment which is a closed system. These control methods are alkaline scrubbing for SO_3 and catalytic converter for N_2O_5. By using catalytic converters (platinum based catalyst) N_2O_5 will be oxidized to N_2. Moreover in alkaline scrubbing method, SO_3 reacts with limestone giving this reaction:

$$CaCO_3 + SO_3 \rightarrow CaSO_4 + CO_2$$
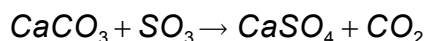
So with these control methods oxides sulfur and nitrogen are removed from the environment releasing the same amount of CO_2. This means that because there is no other pollutant than CO_2 present, the fuel types can be compared by the the amount of heat energy giving out per one mol of CO_2 released into the atmosphere. **From the calculations (see Appendix 2 Table 1) the Heating value : CO_2 ration and thus the efficiency of the fuels are found to be:**

Soma Coal > Beypazarı Coal > Zonguldak Coal > Hexadecane > Dodecane > Octane

In the other situation we assume that no control methods are present in the environment which is a closed system. So there will some sulfur and nitrogen based pollutant released from the combustion reactions of coals used in the experiment. This makes the hydrocarbons more adventageous and efficient as they release only CO_2. **Moreover as the amounts of both N_2O_5 and SO_3 increase with the decreasing C element in the fuel in coals, coal types with more C element present is more adventageous. By using all these facts a comparison of efficiency can be made:**

Hexadecane > Dodecane > Octane > Zonguldak Coal > Beypazarı Coal > Soma Coal

What's more the hydrocarbons used in this project are in liquid state in room temperature. This is another advantage as it easier to transport for these type of fuels from one place to another.

Apart from these there are some limitations to the results of the experiment as it doesn't explain some of the situations that can be encountered in real life. **The most important limitation of this experiment is the unability to obtain any data of incomplete combustion of the hydrocarbons and coal used in this experiment**. If the air present in the environment is not enough for the complete combustion of these fuels, CO will be produced and released into the atmosphere. This air pollutant is much more dangerous than CO_2 because it is a metabolic poison which can be lethal as it binds to hemoglobin and prevents hemoglobin from carrying O_2. **However this situation can be overcome using catalytic converters or thermal exhaust reactors.** Another limitation is caused by the hydrocarbons that doesn't contain any S or N. Because pure O_2 is used in this experiment no SO_3 or N_2O_5 is produced by the combustion reactions of hydrocarbons, however in real life as air is used for the combustion reaction, some sulfur and nitrogen based air pollutant will be formed.

Appendix 1

Experimental Procedure

Materials:

- Bomb calorimeter
- Hydraulic Press
- Pellet
- Circular shaped tablets to make pellets from the samples
- Oxygen gas (17 atm)
- Oxygen cylinder with regulator and hose connetor to fill the oxygen combustion bomb with oxygen gas
- Metal bucket as water reservoir to hold the oxygen combustion bomb
- Oxygen combustion bomb
- Lignite (Beypazarı lignite), bituminous (Zonguldak coal), subbituminous coal samples
- Octane ($CH_3(CH_2)_6CH_3$), dodecane ($C_{16}H_{34}$), hexadecane ($CH_3(CH_2)_{10}CH_3$) samples
- Combustion cup
- Fuse wire (apprx. 10cm)
- Beckmann Thermometer (±0.001)
- Enough water to fill the metal bucket
- Benzoic acid
- Digital scales to weight the samples and the fuse wire

Method:

1. **Preparing powdered coal samples and benzoic acid sample as pellets**
   a. Take samples of the hydrocarbons, coals and benzoic acid and weigh it on a digital scale. The weights of the samples should be roughly between 0.4000-0.8000 gr.
   b. Take a fuse wire about 10 cm and weigh it on the digital scale.
   c. Place the fuse wire in a circular shaped tablet and then fill the tablet with a sample. Two sides of the wire must be swinging from the sides because these will be connected to the electrodes of the ignitor. Be careful when placing the sample as if some falls it will lead to errors in the calculations. **Note:** the powdered sample is is pelletized to make sure that all of it will burn once combustion starts
   d. Place the tablet filled with the sample into the hydraulic press and use the device to do some pressure on the sample to make a pellet out of it.
   e. Repeat the procedures from b to d and make pellets for all the samples including the benzoic acid which will be used to determine the heat capacity of the system
   f. No pellet will be prepared for hydrocarbons used in this experiment as they are in liquid form in room temperature

Picture 1: the hydraulic press used to make a pellet out of the powdered sample

Picture 2: the circular shaped tablet

Pellet

Tablet
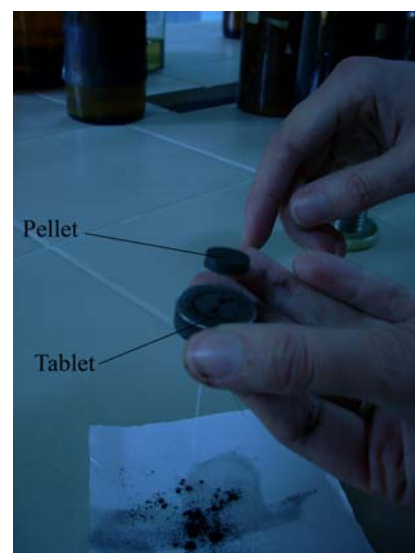
Picture 3: the pellet formed after applying pressure with hydraulic press

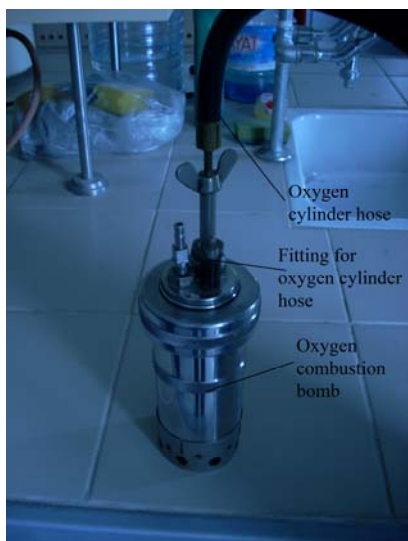2. **Preparing the bomb calorimeter for the experiment**
   a. Place the bomb head in the support stand
   b. Place the combustion cup to the electrode loop as shown in the picture 4.
   c. Wrap the fuse wire that is swinging from the sides of the pellet to the electrodes of the bomb head. Be careful when shaping the fuse wire as it mustn't touch the sides of the metal

cup. **Note**: If the fuse wire touches the sides of the metal cup this will cause a shortcut in the curcuit.

d. Place the pellet into the combustion cup as shown in the picture 4. **Note**: For hydrocarbons just place the liquid in the combustion cup

e. Remove the bomb head from the support stand

f. After removing place head on the bomb body. Be careful not to disturb the pellet or the fuse wire. This might cause some errors in the calculation and the progress of the experiment. Then screw the cap onto the bomb body and make sure you tighten it.

g. Adjust the regulator of the oxygen cylinder to 17 atm.

h. Place the hose of the oxygen cylinder on the fitting of the bomb head as shown in the Picture 5. Tighten the hose well to the fitting or else it might leak some gas.

i. Purge the bomb 2-3 times at 17 atm.

j. Fill the bomb with oxygen at 17 atm. Then release the pressure. **Note:** The bomb is filled with pure oxygen in order to ensure that a full combustion reaction occurs.

Picture 4: the preparation of the bomb head.

k. Fill the water bucket (water reservoir) with enough water to cover the bomb as shown in the picture 6.

l. Place the bomb in the water bucket. Check if any bubbles are being produced. If there are bubbles, it means that the bomb leaking, so the procedure should be stopped with the bomb being released and repressurized.

m. Place the bucket and the bomb right inside the bomb calorimeter.

Picture 5: the hose of the oxygen cylinder placed to the fitting of the oxygen combustion bomb

Picture 6: the water reservoir and the oxygen combustion bomb placed in it

n. Be sure to close the cover of the calorimeter after putting the bomb and the bucket inside it.
o. Place the thermometer to its opening on the cover of the calorimeter.

3. **Starting the ignition and observing the temperature change**
    a. After preparing the bomb calorimeter and the apparatus check if everything is ok. If so, press the black button on the panel of the calorimeter. This button will start the ignition process.
    b. Check if the light of the led on the panel of the calorimeter turns on and then off for second or so. This means that there is a current passing through the fuse wire. If there is no light check if the fuse wire is connected properly to the electrode.

Picture 7: the calorimeter

    c. When the light of the led turns off this means that the combustion reaction has been completed.
    d. After the reaction has been completed there will be some changes in the temperature of the calorimeter system. These changes must be observed in order to calculate the enthalpy of the sample.
    e. In order to observe the temperature changes look through the magnifying lens which is on the calorimeter to the Beckmann thermometer. Note: As the Beckmann thermometer has a uncertainty of ±0.001 only way to see the values is to look through a magnifying lens.
    f. The temperature changes per a minute must be noted as data until the calorimeter cools down and the temperature stops changing.
    g. Then the oxygen combustion bomb and the water bucket is removed from the calorimeter.
    h. After opening the bomb the fuse wire is taken out and its weight is measured on a scale. This is used in the calculation of enthalpy.

4. **Finding the heat capacity of the bomb calorimeter system**
    a. Prepare the bomb calorimeter and the apparatus using benzoic acid as the sample pellet
    b. After preparing everything the ignition must be started and the temperature changes must be observed as told in the point 3.
    c. When the reaction is completed and all the data is collected ΔT must be calculated. As the literature value of the energy released by this reaction is 6.32 kcal/g the heat capacity of the system can be calculated with this formula:

$$\text{Heat capacity of calorimeter} = \frac{\text{energy released by the reaction}}{\Delta T} = \frac{6.32}{\Delta T}$$

Appendix 2

Fuel Types	Amount of CO_2 released from combustion reaction (mol/g)	Amount of CO_2 released from catalytic converter (mol/g)	Amount of CO_2 released from alkaline scrubbing (mol/g)	Total amount of CO_2 present in the environment (mol/g)	$\frac{Heating\ Value}{CO_2}$ ratio
Zonguldak	0.0750	3.61×10^{-4}	1.56×10^{-4}	0.0760	117627.6316
Beypazarı	0.0510	7.39×10^{-4}	0.0020	0.0540	125020.3704
Soma	0.0270	0.0011	0.0024	0.0305	135315.0820
Octane	0.0701	-	-	0.0701	17245.3637
Dodecane	0.0705	-	-	0.0705	25669.7870
Hexadecane	0.0707	-	-	0.0707	42044.6959

Table 1: amounts of CO_2 released from the reactions of control methods and the heating value : CO_2 ratio

Alican Salor
001129–057

References

1) McLamb, Eric. "The Industrial Revolution and Its Impact on Our Environment". May 19, 2008. <http://www.ecology.com/archived-links/industrial-revolution/index.html>

2) Montagna, Joseph A. "The Industrial Revolution". <http://www.yale.edu/ynhti/curriculum/units/1981/2/81.02.06.x.html

3) http://en.wikipedia.org/wiki/Petroleum>

4) Zumdahl, Steven-Zumdahl, Susan.Chemistry Sixth Edition, pg 250, 253, 254, 270, 271

5) "Bomb Calorimetry". <http://www.chem.hope.edu/~polik/Chem345-2000/bombcalorimetry.htm>