PREDICTION OF CALORIFIC VALUE OF INDIAN COALS BY ARTIFICIAL NEURAL NETWORK

A THESIS SUBMITTED IN PARTIAL FULFILLMENT

OF THE REQUIREMENTS FOR THE DEGREE OF

BACHELOR OF TECHNOLOGY

IN

MINING ENGINEERING

By

KAILASH SEERVI

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DEPARTMENT OF MINING ENGINEERING
NATIONAL INSTITUTE OF TECHNOLOGY
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National Institute of Technology, Rourkela

C E R T I F I C A T E

This is to certify that the thesis entitled "**Prediction of Calorific Value of Indian Coals by Artificial Neural Network**" submitted by **Sri Kailash Seervi** (Roll No. 111MN0476) in partial fulfillment of the requirements for the award of Bachelor of Technology degree in Mining Engineering at the National Institute of Technology, Rourkela is an authentic work carried out by him under my supervision and guidance.

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University/Institute for the award of any Degree or Diploma.

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ABSTRACT

The experimental determination of calorific value of solid fuels is a cost intensive process, as it requires spatial instrumentation and highly trained analyst to perform the experiments, whereas proximate analysis data can be obtained easily using an ordinary muffle furnace compared to calorific value. Regression analysis and artificial neural network analysis methods have been introduced to simplify the task and also reduce the cost of analysis. An endeavor has been made in this present study to access the applicability of these correlation and artificial neural network with a spatial emphasize on Indian coals. Correlation have been created using simple linear regression and multivariable linear Regression analysis based on proximate analysis of data sets. Artificial neural network model is also designed to predict the gross calorific value of coals belonging to different Indian coal fields.

59 samples were collected from different coal fields of India including the South Eastern Coalfields (SECL), Singareni Collieries Company Limited (SCCL), Central Coalfields limited (CCL), Mahanadi Coalfield Ltd. (MCL), Eastern Coalfields Limited (ECL), North Eastern Coalfield Limited (NECL), Jindal Steel and Power Limited. The intrinsic properties were determined by carrying out proximate analysis and gross calorific value (GCV) by using bomb calorimetry. The results for intrinsic properties and the gross calorific value are given in table 1.

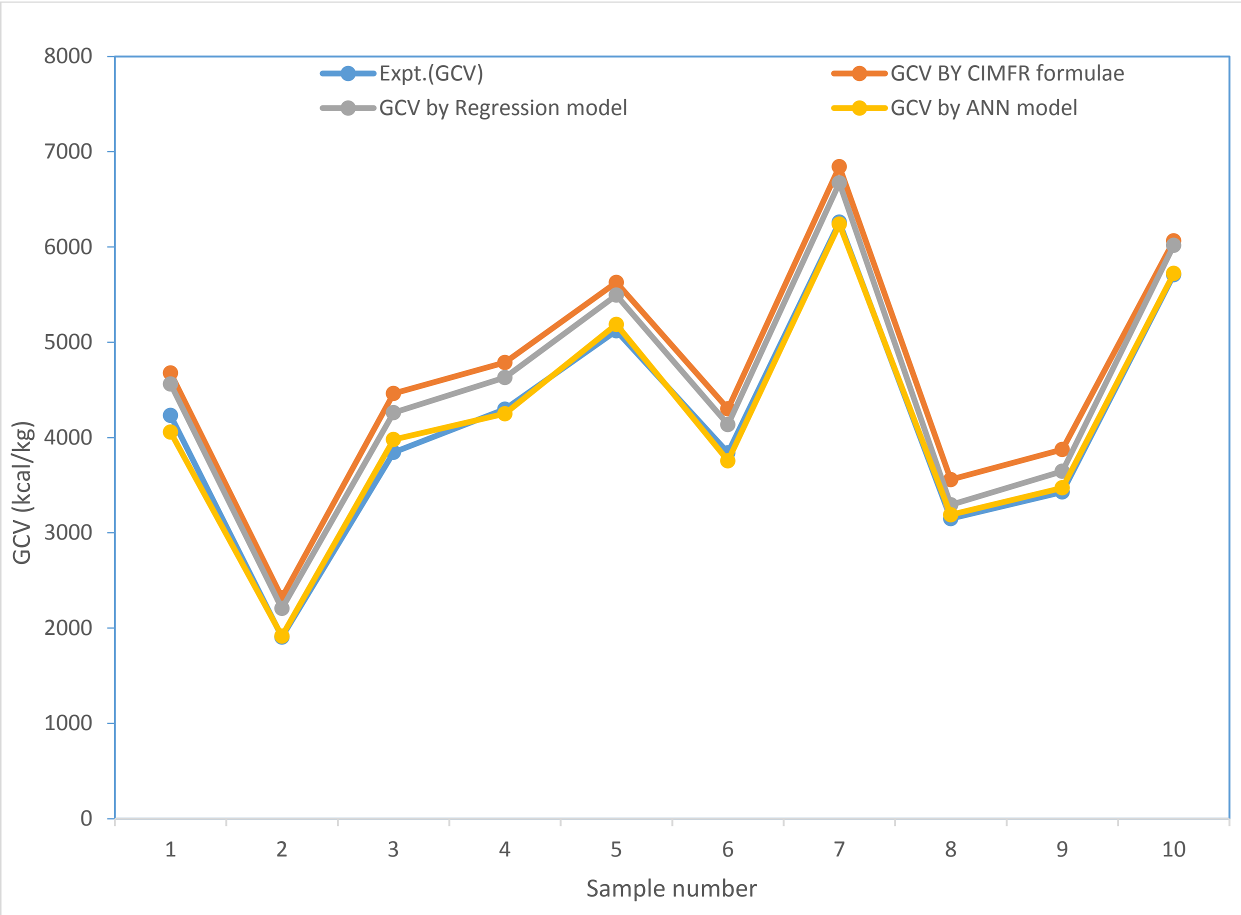
Correlation analysis was carried out to analyze the individual effect of moisture, volatile matter, ash and fixed carbon on the gross calorific value (GCV). It is observed that moisture , ash have adverse impact and reduce the gross calorific value whereas volatile matter ,fixed carbon have positive impact and increase the gross calorific value(GCV). Present study also compares the experimental results to formulae given by CMFRI and model created by using multivariable linear regression and artificial neural network. The formulae developed by multivariable linear regression is

GCV= 7115.197 - 123.971*M - 81.3121*A + 20.7421*FC,

Where GCV in kcal/kg and moisture, ash, fixed carbon in air dried percentage basis.

In the present study, 49 samples were used to develop the regression model and 10 were used to authenticate and compare the results by various models. The comparison of the results of

calorific value determined by CIMFR formulae, regression, model and ANN model with that of the experimentally determined GCV has been presented in the figure below.



Comparison of GCV determined by different methods

It may be observed that all the three models predict the calorific value fairly accurately. However, the ANN model gives a better prediction than the other methods. Therefore, prediction of gross calorific value by ANN model could be a viable option than experimentation in the laboratory. The ANN model considers the intrinsic properties determined by proximate analysis as input parameters, which is a routine task in the field as these are required to determine the grade of coals and hardly demand any costly experimental setup.

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CHAPTER: 1

INTRODUCTION

1. INTRODUCTION

1.1 GENERAL

Coal is the world's most abundant and widely distributed fossil fuel. It is a global industry that makes a significant economic contribution to the global economy. Coal is mined commercially in more than 50 countries and used in more than 70. Annual world coal consumption is about 5,800 million tons, of which about 75% is used for electricity production. This consumption is projected to nearly double by the year 2030 to meet the challenge of sustainable development and a growing demand for energy.

The International Energy Agency (IEA) predicts that world energy demand will grow around 60% over the next 30 years, most of it in developing countries. China and India are very large countries in terms of both population and land mass, and both have substantial quantities of coal reserves. Together, they account for 70% of the projected increase in world coal consumption. Strong economic growth is projected for both countries (averaging 6% per year in China and 5.4% per year in India from 2003 to 2030), and much of the increase in their demand for energy, particularly in the industrial and electricity sectors, is expected to be met by coal.

For power plant and industrial application, it is a common practice to assess the quality of coals by using calorific value, proximate analysis and ultimate analysis. Calorific value is the amount of heat evolved by their complete combustion and experimentally it is determined by bomb calorimeter, this method of determination is cost intensive and requires sophisticated equipment and also trained chemist similarly ultimate analysis of coal also needs very expensive equipment and trained analyst, while moisture(M),ash(A),volatile matter(V_M),and fixed carbon(F_C) are determined easily by proximate analysis of coal by using simple muffle furnace and it is relatively cheaper than the bomb calorimeter and moderately trained chemist can be performed.

Energy demand of the entire world is increasing recently and are mostly compensated by the fossil based fuels like natural gas, fuel oil and coal. Coal is very crucial energy sources for many countries, among the fossil fuels, which produce heat and electrical power by distinct technologies to fulfill our daily life requirements. Hence prediction of coal quality is an essential task and mainly depend on knowledge about its chemical and physical constitution.

In present study, a model is developed by using multivariable linear regression. Out of 59 data samples 49 data samples are used for model development and 10 samples data for validation or checking purpose. Simple linear regression also used to analyze the individual effect of moisture, ash, volatile matter and fixed carbon on calorific value of coal. Neural network is a new mathematical method introduced and widely used in research areas of industrial processes. Artificial neural network (ANN) is an empirical modeling tool, inspired by behavior of biological neural structures. Neural networks are powerful tools that have abilities to identify underlying highly complex relationships and connections from input–output data.in present study artificial neural network model developed using 49 samples and 10 samples use for validation.

1.2 OBJECTIVES

Keeping the above problem in mind, the objectives of the current work has been outlined as:

- Assessment of different parameters that affect the calorific value of coal.
- Determination of intrinsic properties of the coal samples using proximate analysis and bomb calorimetry.
- Development of the formulae for prediction of gross calorific value of coal by proximate analysis data using multivariable linear regression.
- Development of the artificial neural network model for prediction of gross calorific value and comparison of multivariable regression and ANN models.

CHAPTER 2

LITERATURE REVIEW

2. LITERATURE REVIEW

Elder (1983) studied the use of PerkinElmer thermo gravimetric instrumentTGS-2, under the control of the system-4 microprocessor for the automatic proximate analysis of solid fossil fuels and related matter. Classical proximate analysis is time consuming and tedious and does not lend itself to the speedy determination of one sample and required sample size (10 g) are relatively large.Thermogravimetric analysis (TGA) is a simple, speedy and yield precise, accurate and required sample of small sizes (1 to 10 g) range and it has utility when results on one sample are immediately required .Three different programs were used in this study. Each step was defined in term of a fixed time interval. In step 1 system was held at approximately 30^0 for5 minute, which cause the sample to lose absorbed moisture.in step 2 the sample was heated to 110^0 in 30 second and held isothermally for a further 4.5 minute, to cause the removal of absorbed water. Then the sample is heated over a 5 minute period at the temperature either 900^0 or 950^0 and held isothermally at this upper limit for further 5 minutes to allow the removal of volatile matter.

Kok et al. (2001) carried out the experimental analysis of coal thermal behavior. They took 10 coal samples of different origin for their study. They applied complex thermal analysis techniques (TG/DTG, DTA) for the determination of calorific value of coals of distinct origin. The main analysis of coal using thermal analysis contain the characteristics of higher pressure application to coal hydrogenation, catalytic effects by inorganic substances, combustion, pyrolysis and kinetic study. Thermal analysis is a convenient tool to determine the proximate analysis of the coal samples giving comparable results to those of ASTM standard methods. Coal samples were prepared using ASTM standards and their particle size were < 60 mesh.TG/DTG and DTA curves were obtained using atmosphere-nitrogen, air of flow rate -50 ml/min, 10 mg sample, heating rate-100/min and temperature range-20 to 800^o C .experiment results by thermal analysis technique are discussed with adiabatic bomb calorimeter using the standard ASTM method.

Majumdar et al. (2008) carried out the experiments of 250 coal samples taken from coalfield of central India (well known as south eastern coalfield limited SECL).HHV (high heating values) and proximate analysis of coal samples have been carefully determined. Moisture, ash, volatile matter and fixed carbon were determined using ASTM-D5142 proximate analyzer model TGA-

601 by thermo-gravimetric analysis (TGA).Bomb calorimeter model AC-350 was used for determined HHV of these samples following ASTM procedure. Out of 250 data, 164 were selected to generate the correlation and 86 were kept separate for validation purposes. For the model development multiple linear regression has been adopted. It helps in the modeling relationship between two or more explanatory variables. The results obtained were carefully examined the impacts of moisture, ash, volatile matter and fixed carbon on the HHV of coal. It were observed that moisture and ash have negative effect and volatile matter and fixed carbon have positive impact on the HHV of the coals. They proposed an equation by using multiple linear regression analysis and suggested that there is a genuine basis to accept it for HHV estimation of coal because it deals with all the major variables affecting HHV.The average absolute error between predicted and experimental data was found quite low and established the validity of the proposed equation.

Mesroghli et al. (2009) carried out the study of assessment of properties of 4045 US coal samples from 25 states with references to GCV and possible variation with ultimate and proximate analysis using multivariable regression, SPSS software package and ANNS, MATLAB structure package. Calorific value is very important property and indicated the useful energy content by coal and its value as a fuel. A number of equations have been developed for the prediction of gross calorific value (GCV) using the proximate or ultimate analysis. The database include the determined proximate and ultimate analysis and calorific as received basis. They Compared the predicted GCV and actual GCV and concluded that the input set "C, H (exclusive of moisture), N, O (exclusive of moisture), moisture and ash can be used as the most reliable inputs for the prediction of gross calorific value of coal using multivariable regression and the deviation and error from the experimentally concluded GCV in ANN is not much better or different from regression.

Verma et al. (2010) used the study for intelligent prediction of heating value of coal and the data used to predict GCV was taken from the U.S. Geological Survey coal quality database open fire report 97-134.Heating value or gross calorific value (GCV) of a sample is one of the most important properties which defines the energy of fuel and mainly determined by bomb calorimeter in the laboratory but these methods are expensive and time consuming. Multivariable regression and co-active neuro-fuzzy interference system (CANFIS) were used for the prediction of GCV, considering the all major constituents of the proximate and ultimate analysis as input parameters. Correlation had been developed using multivariable regression analysis that were simple to use based on the ultimate and proximate analysis of data sets from 25 different states of USA.CANGIS backed by genetic algorithm model was designed to predict the GCV of 4540 US coal samples. Optimization of the network architecture was done using a systematic (genetic algorithm) approach. The network was trained with 4371, cross validation with 100 and predicted with rest 69 dataset. The predicted results were compared with observed values. Mean average percentage error was found to be negligible and the generalization capability of model was established to be excellent. The results of that investigation provided the functional and more information for prediction of GCV of any type of coal in USA.

Sharma et al. (2012) carried out the study of coal samples collected from the different north eastern Indian coalfields (Assam, Meghalaya, Nagaland and Arunachal Pradesh) by adapting standard sampling methods. Petrographic study, Proximate analysis and sulphur analysis have been done by using proximate analyzer(TGA 701,leco,USA)and 144 DR sulphur determinator and the percentage of oxygen was calculated by difference. Calorific values of coal samples had been determined by using automatic bomb calorimeter(LECO AC-350).The relationship between gross calorific value(GCV) and macerals contents of these coal samples had been investigated by multi variable linear regression analysis. Regression analysis is the statically tool used to investigate the relationship between variables. The maceral analysis indicated that north eastern coal samples had high vitrinite contents (80.07%), moderate to low liptinite (10.23%) and a low inertinite (9.3%).From their investigation, the inter correlation between GCV of coals and maceral analysis showed that with the increase in interinite contents in coal, there is decrease in GCV and the higher vitrinite and liptinite in coal can result in higher GCV.

Krishnaiah et al. (2012) carried out the study for around 150 lab analysis data of coal and both proximate and ultimate information used to train and test the ANN model. Ultimate analysis is the process to know elemental composition of coal. The ultimate analysis is expensive, time taking and also cumbersome in nature but at the power plants only the gross level coal composition are estimated which is known as proximate analysis. The elemental compositions were estimated by using standard empirical formulae based on the gross level compositions of coal. Relationship between the elemental composition and gross level composition was nonlinear. To achieve better performance of boiler and control on the boilers, accurate information of elemental composition is required. So they suggested a method to compute ultimate analysis by proximate analysis using artificial neural network model (ANN). The prediction of ANN model and empirical models were compared and found that ANN prediction is good with lab data than the predictions of empirical model.

Yerel et al. (2013) studied the coal quality parameters such as ash content, calorific value and moisture content, 79 borehole samples were collected from western turkey. In their study, they predicted calorific values using linear regression analysis using both simple linear regression and multiple linear regression analysis and models developed for predictions. Linear regression was applied to determine the relationship between dependent variable calorific value and ash content, moisture as independent variables. The aim of regression analysis was to determine the values of parameters for a function that causes the function to best fit a set of data observations provided and it was conclude that calorific values can estimated using a multiple linear regression model.

Upadhyay (2014) investigated the physical and chemical properties of coal in Korba district for assessment of coal quality, in order to check it’s suitability for thermal power station, by collecting samples from Gerva coal mines. Three different coal samples were collected from different areas of Gerva coal mines and analyzed for ultimate, proximate and calorific value as per standard methods and From overall analysis and according to useful heat value(UHV) of coal samples, they were concluded that the grade of Gerva coal was “F” and very useful for coal based thermal power station.

CHAPTER: 3

EXPERIMENTAL INVESTIGATIONS

3. EXPERIMENTAL INVESTIGATIONS

3.1 Sampling

Sampling is the procedure of acquiring a representative set of data from the original population. The reason of collecting and preparing a coal sample is to provide a test specimen which when analyzed and study will provide the test results illustrative of the lot sampled. Coal is a very heterogeneous mass in nature and most difficult material to be sampled because of its varying composition from combustible to non-combustible in a single seam. In India, this change happens with depth, length and breadth of the seam in the same mine. Sampling of coal and analysis is essential to check for the quality of coal where coal seams to be mined or under production and also very important for the coal reserve estimation. Sampling is essential for many reasons such are part of reserve estimation, part of mine development and quality check of part of coal seams. Coal sampling and analysis estimate whether coal can be sold as a cocking coal, prime coal, metallurgical coal or low grade coal. Coal samples were collected from different mines in small quantities to analyze the constituents of the whole seam.

Coal sampling methods:

Samples can collected from coal outcrop, from exposed seam in opencast or deep mine, chips or cores from drill holes and different sampling methods are:

1. Grab samples
2. Pillar samples
3. Core samples
4. Channel samples
5. Chip samples
6. Bulk samples

Grab sampling: Generally this method of obtaining coal is not widely used because this method forces us for bias selection that means we used to collect those samples which attracts us instead of our requirement like bright coal gains more attention. However, grab samples can help us to determine the vitrinite reflectance of coal which indicates the coal rank.

Channel sampling: Channel sampling are representative of the coal from which they are collected. If the coal sample which is collected is exposed in air then the outcrop must be cleaned and a layer from sample is taken out to expose as fresh section.

Steps of channel sampling

Channel Sampling is carried out in a series of steps:

1. Preparation of surface: The surface of coal is cleaned by using scrubbers or brushes in order to remove dirt, dust, oxidized part of coal which is exposed to air and other soluble salts. Also a layer of about 10 cm thick from sample is taken out to expose as fresh section.

2. Demarcation of the channel: After cleaning the surface, a channel is marked by drawing two parallel lines 12-15 cm apart using chalk or paint.

3. Cutting the channel: In case of soft coal mines channel cutting is done by hand picks and in case of hard coal generally a light weight air operated drill machine is used. In case of underground mines drill machines are used to cut channels in case where more no of samples are to be collected in a single shift.

4. Collection the sample: A sheet of canvas is spread on the floor to collect the coal chips as they fall from seam.

5. Labelling the sample: collected the coal sample is wrapped in the canvas sheet and marked. Then the marked canvas is brought out of the mine.

Bulk Sampling: Bulk Sampling Method is the simplest samples collecting method. In this method a large mineralized rock around fifty tones is removed and is selected to represent of the potential ore body for mineral processing tests. It is used where schematic sampling procedure is unable to provide a representative scale. Large scale sampling or bulk sampling removes the adverse effect of irregular distribution of small value and then a small part of the sample is considered for the experimental purposes.

In the present study, 59 samples were collected from different coal fields of India following the channel sampling procedure. The samples belong to South Eastern Coalfields (SECL), Singareni Collieries Company Limited (SCCL), Central Coalfields limited (CCL), Mahanadi Coalfield Ltd. (MCL), Eastern Coalfields Limited (ECL), North Eastern Coalfield Limited (NECL), Jindal

Steel and Power Limited. The collected samples from different mines are brought to the laboratory for analysis. It is crushed to smaller pieces using crusher. Coning and quartering procedure is done in order to get a small representative sample of the entire coal seam. Finally the samples is screened to different size of - 212 (micron), -100 to 200, -100 etc. Then the samples are stored and sealed for further analysis.

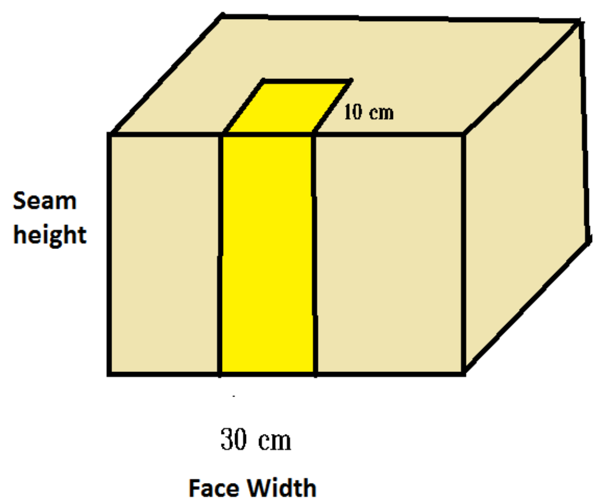

Figure: 3.1 channel sampling

Core sampling: This technique is used in underground or undersea exploration. A core sample is of cylindrical shape which is taken out using special drills and brought to the surface for analysis. This types of sample is needed to determine bulk properties of rock like its porosity and permeability, or to investigate the peculiar features of a given zone of strata.

The collected samples from different coalfields were brought to the laboratory. It was then crushed to smaller pieces. Coning and quartering procedure was done in order to get a small representative sample of the entire coal seam. Finally the samples were grounded and screened (sieving) to different size of - 212 (micron), -100 to 200, -100 etc. according to the desired requirement of the experiment. Then the samples were stored in sealed packets for further analysis process. It was placed in moisture oven to make it air dry.

To carry out the experimental study, coal samples were collected by channel sampling method as described in IS 436 Part I/Section I - 1964. The intrinsic properties of the collected samples were determined by proximate analysis and bomb calorimetry experiment.

3.2 Proximate analysis (IS 1350 part I -1984)

Moisture:

Coals are extracted from the ground and have some amount of moisture with them. Heating of coal at a temperature of 100^0C causes a loss of weight due to drying of coal that moisture content is defined as inherent moisture. The moisture content of coals ranges from about 5% to 70%. Moisture is an unwanted constituent of coals as it reduces the calorific. The inherent moisture is due to the inherent hygroscopic nature of coal.

Experimental procedure:

Experimentally moisture content of the coal samples is find out by taking 1g of fine powder (-212 μ) of air-dried coal sample in a watch glass. This is then placed inside an oven at temperature of 108±2 °C. Sample is kept in the oven for 1.5 hours and is then taken out with a pair of hand gloves. The sample is then cooled in a desiccator for about 15 minutes and then weighed. The loss in weight is noted as moisture.

The calculation is by following formula,

Where,

X = weight of empty crucible, g.

Y = weight of crucible + coal sample before heating, g.

Z = weight of crucible + coal sample after heating, g.

Y - X = weight of coal sample, g.

Y- Z = weight of moisture, g.

Figure: 3.2 Muffle Furnace for Ash Content & Volatile Matter Determination and Oven for Moisture Content Determination

Volatile Matter:

Volatile matter includes all those components of coal, except for water, which are liberated when heated at high temperature in the absence of oxygen. Volatile matter increases the risk of spontaneous combustion of coal. When coal is heated at high temperature thermal decomposition of various constituents of coal takes place hence reduces the mass which is used in determination of Volatile matter.

Experimental Procedure

An empty silica crucible is taken and weighed. 1g of coal sample is taken of -212μ size. Coal and crucible is weighed together and placed inside a muffle furnace with the lid covering the crucible maintained at temperature 925±5 °C. The sample is heated for exactly seven minutes, after which the crucible is removed and allowed to cool in air, then in a desiccator and weighed again. The calculation was done as per the following.

The calculation is by following formula, Where,

Where X = weight of empty crucible, g

Y = weight of crucible + coal sample before heating, g

Z = weight of crucible + coal sample after heating, g

M = Moisture content

Y-X = weight of coal sample, g

Y- Z = weight of volatile matter + moisture, g

Ash Content:

Ash is the non-combustible residue formed from the inorganic or mineral components of the coal. Indian coals are of drift origin. The procedure followed for determination of ash content is follows. An empty silica crucible is taken and cleaned by heating it in furnace for 800^0C and allowed to cool and weighed. 1g of coal sample is taken of -212µ size. Coal and crucible is weighed together and placed inside a muffle furnace maintained at temperature 450^0C for 30 minutes and then temperature of the furnace is raised to 850°C for 1 hour. After which the crucible is removed and allowed to cool in a desiccator and weighed again.

The calculation is by following formula,

Where,

X = weight of empty crucible in grams

Y = weight of coal sample + crucible in grams (Before heating)

Z = weight of coal sample + crucible in grams (After heating)

Y - X = weight of coal sample, g

Z - X = weight of ash, g

Fixed Carbon

It is determined by subtracting the sum of all the above three parameters from 100% and is given as Fixed Carbon,

$$FC = 100 - (M + V + A)$$

Where, M: Moisture content

V: Volatile matter content

A: Ash content

The results of proximate analysis has been presented in Table 3.1.

Table 3.1: Results of Proximate Analysis:

Sl. No.	**Moisture (%)**	**Volatile Matter (%)**	**Ash Content (%)**	**Fixed Carbon (%)**
1	11.13	25.19	38.46	25.22
2	14.29	31.25	16.27	38.19
3	7.25	23.9	40.5	28.35
4	8.97	29.49	22.88	38.66
5	10.02	26.06	31.57	32.35
6	11.32	29.81	21.8	37.07
7	9.12	33.51	8.37	49
8	8.72	25.14	13.75	52.39
9	6.74	26.14	34.89	32.23
10	7.64	22.13	37.02	33.21
11	5.0	24.01	32.4	38.59
12	4.88	24.17	38.87	32.08
13	1.9	33.08	16	49.02
14	0.6	22.32	10.73	66.35
15	10.0	32.27	18	39.73
16	7.67	29.83	18.88	43.62
17	14.39	29.31	12.76	43.54
18	3.18	20.26	55.24	21.32

19	3.02	20.43	53.7	22.85
20	5.0	26.5	17.0	51.5
21	6.5	32.0	23.5	38.0
22	4.5	32.0	12.0	51.5
23	2.98	34.17	12	50.85
24	5.0	32.33	34	28.67
25	5.05	22.49	48.5	23.96
26	1.0	21.89	34.33	42.78
27	1.0	24.62	26.5	47.88
28	5.97	35.49	26.49	32.05
29	1.0	22.54	34.16	42.3
30	1.0	22.11	34.33	42.56
31	1.5	43.03	5.37	50.1
32	2.96	19.27	54.54	23.23
33	2.68	19.63	56.82	20.87
34	2.91	19.88	56.07	21.14
35	12.82	36.75	10.28	40.15
36	6.97	23.69	45.25	24.09
37	3.07	16.72	61.99	18.22
38	2.59	17.26	59.77	20.38
39	12.64	36.47	10.54	40.35
40	13.13	36.18	10.59	40.1
41	8.06	25.3	40.09	26.55
42	13.91	35.97	9.85	40.27
43	6.09	22.1	52.99	18.82
44	13.04	39.56	9.99	37.41
45	6.29	23.74	47.09	22.88
46	6.92	29.19	32.55	31.34
47	2.82	16.91	63.69	16.58
48	2.84	17.01	61.26	18.89
49	2.56	16.29	63.96	17.19

50	4.38	22.99	34.46	38.17
51	3.09	12.46	61.51	22.94
52	4.98	26.61	35.82	32.59
53	3.75	25.05	34.27	36.93
54	5.0	28.04	23.41	43.55
55	2.96	22.98	40.65	33.41
56	7.02	36.06	7.38	49.54
57	2.29	24.3	49.58	23.83
58	4.07	24.98	43.47	27.48
59	5.5	26.0	18.0	50.5

3.3 Determination of Calorific Value

Calorific Value: The calorific value of the any fuel is the quantity of heat produced by its complete combustion at the constant pressure and under normal (standard) conditions (to 0C and under a pressure of 1,013 mbar).Due to the combustion process it generates water vapour and certain techniques may be utilized to recover the quantity of the heat contained in this water vapour by condensing it.

Gross Calorific Value (GCV) or Higher Calorific Value or Higher Heating Value (HHV):

Water of combustion is completely condensed and here the heat contained in the water vapour is recovered.

Net Calorific Value (NCV) or Lower Calorific Value or Lower Heating Value (LHV):

The products of combustion contains the water vapour and here the heat in the water vapour is not recovered and utilize.

Table 3.2: Grading of non-coking coal base on heating value of coal

Grade of coal	Useful heat value(kcal/kg)
A	>6200
B	5601 to 6200
C	4941 to 5600
D	4201 to 4940
E	3361 to 4200

F	2401 to 3360
G	1301 to 2400

Bomb calorimeter

Bomb calorimeter is an arrangement consist of a hollow cylindrical vessel called bomb made up of stainless steel. The cylinder has an air tight cover which is screwed over the cylinder. The cover consist of three terminals. One for the filling oxygen into the bomb and the other two terminals are for passing electric current ignite the coal by producing spark. After the oxygen is forced into the bomb the terminal is closed.

The whole arrangement is then kept inside a water jacket containing water of a known amount. A mechanical stirrer is provided to mix the water inside jacket to maintain an even temperature distribution in water. A thermocouple is provided for recording the temperature of water.

Figure 3.3: Digital Bomb Calorimeter

Experimental Procedure

1gm of coal is weighed in the digital balance and the reading imported to the bomb calorimeter using start pre-weight button and stored adjacent to the name of sample. Coal was then placed in the small crucible and fixed in the arrangement provided in the cover of bomb. A piece of nichrome wire was cut and attached to the two rods below the cover such that the wire is in contact with coal. The whole arrangement was carefully screwed over the bomb and oxygen line was attached over the valve on the cover. Then Oxygen fill button was pressed and oxygen was filled in the bomb. After that the bomb was carefully placed inside the water jacket. The bomb is placed in such a way that it does not come in contact with the stirrer. Then the leads are attached to the two terminals provided on the cover. The lid of machine is closed and the Start button is pressed. After sometimes the machine will ignite the coal and display the Gross Calorific Value on screen.

Table 3.3: Experimental Gross calorific value (GCV) of coal samples:

Sample no.	Calorific Value (Kcal/kg)
1	3463.1474
2	5156.3208
3	3512.8162
4	4987.3952
5	3999.0795
6	4896.3036
7	6377.2046
8	6147.502
9	3802.3586
10	4112.8205
11	4027.3616
12	3800.6971
13	6697.9463
14	7315.2393
15	5119.7828
16	5216.9496

17	5684.6029
18	2693.26
19	2870.4
20	5931.0413
21	4782.1141
22	6290.1933
23	6691.4788
24	4316.278
25	3156.5704
26	5337.3588
27	6295.6121
28	5015.3253
29	5426.9737
30	5121.9532
31	8075.0511
32	2819.22
33	2585.15
34	2581.11
35	5399.88
36	3105.24
37	1945.34
38	2237.39
39	5350.35
40	5298.07
41	3508.35
42	5325.2
43	2387.38
44	5229.55
45	2936.8
46	4410.78

47	1994.67
48	2063.32
49	1958.61
50	4232.1224
51	1905.0932
52	3844.6028
53	4296.98
54	5120.5295
55	3839.435
56	6260.7414
57	3148.7752
58	3429.1988
59	5708.4967

CHAPTER: 4

MODEL DEVELOPMENT

4. MODEL DEVELOPMENT

4.1 Model Development by Regression Analysis

Linear Regression: Linear Regression is a statically approach for modeling the relationship between a scalar dependent variable (Y) and one or more explanatory variables or independent variable donated by X. The case of one explanatory variable is known as simple linear regression and for more than one explanatory variable, the process is called multiple linear regression.

In the linear regression process, data are modeled using linear predictor function and unknown model parameters are estimated from the data, such models are called linear models.

Simple linear regression:

It is the least squares estimator of a linear regression model with a single explanatory variable.

Suppose there are N data points ((X, Y), i=1, 2……..N).the function that describes X and Y is:

$Y_i = A + BX_i + e_i$

And here the goal is to find out the equation of straight line

$Y_i = A + BX_i$

Which provide the "best" fit for the data points and best will best will be understood in the least squares approach and a line that minimizes the sum of squares residuals of the linear regression model.

Multivariable linear regression:

Multivariable linear regression model attempts to the relationship between two or more explanatory variables and a response variable by fitting a linear equation to observed data. Every value of the independent variable x is associated with a value of the dependent variable y.

Formally, the model for multiple linear regression, given observation, is

$Y_i = B + B_1X_{i1} + B_2X_{i2} + \ldots\ldots\ldots\ldots\ldots + B_pX_{ip} + e_i$

For i = 1, 2……, n

In the least square model the best fitting line for the observed data is calculated by minimizing the sum of the squares of the vertical deviations from each point to the line. The deviations are firstly squared then summed, there are no cancellations between positive and negative values.

By using the 49 experimental data of proximate analysis and gross calorific value of coal in present study formulae were developed by using multivariable linear regression and 10 samples were used for checking purpose. Developed formulae given by:

GCV = 7115.197 - 123.971*M - 81.3121*A + 20.7421*F

Where the M, A, F denote the moisture, ash content, fixed carbon percentage air dried basis, respectively. The comparison of the predicted GCV by regression and model and that of the experimentally determined value has been presented in Table 4.1.

Table 4.1: Experimental GCV and Predicted GCV by Regression Model

Sl. No.	Experimental GCV(kcal/kg)	Predicted by Regression(kcal/kg)	Difference
1	4232.1224	4561.919	329.796991
2	1905.0932	2206.446	301.353003
3	3844.6028	4261.212	416.609217
4	4296.98	4629.75	332.769586
5	5120.5295	5495.149	374.619694
6	3839.435	4135.902	296.467496
7	6260.7414	6672.408	411.666536
8	3148.7752	3294.136	145.360825
9	3429.1988	3645.995	216.796221
10	5708.4967	6017.22	308.72355

4.2 : Model development by Artificial Neural Network

Artificial neural networks (ANNs) are a family of statistical learning algorithms inspired by the biological neural networks (the central nervous systems of animals, in particular the brain) are used to estimate functions that can depends on large number of inputs and are generally unknown. Artificial neural networks are generally presented as system of interconnected “neurons” which can able to compute values from inputs, and are capable of machine learning as well as pattern recognition.

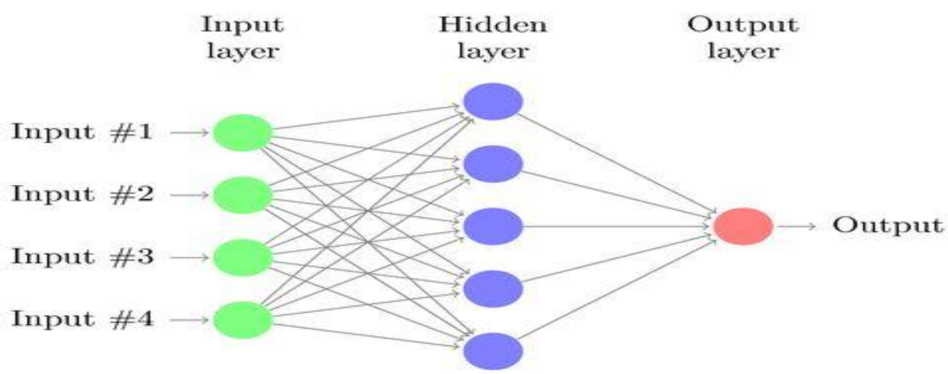

Figure 4.1: Architecture of Artificial Neural Network Model

In the present study for the prediction of gross calorific value of coal 49 coal sample data including proximate analysis and calorific value used for artificial neural network model development and 10 samples were used for the checking purpose. Those 10 samples gross calorific value were predicted and compare with the experimental gross calorific value.

For the ANN Model development ANN tool of MATLAB software used. Feed forward neural network is a biologically inspired classification algorithm. It consist of a (possibly large) number of simple neuron-like processing units, organized in layers. Every unit in a layer is connected with all the units in the previous layer. These connections are not all equal, each connection may have a different strength or weight. The weights on these connections encode the knowledge of a network. Often the units in a neural network are also called nodes.

Data enters at the inputs and passes through the network, layer by layer, until it arrives at the outputs. During normal operation, that is when it acts as a classifier, there is no feedback between layers. This is why they are called feed forward neural networks.

The comparison of the predicted GCV by ANN model and that of the experimentally determined value has been presented in Table 4.2.

Table 4.2: Experimental GCV and predicted GCV by ANN

Sl. No.	Experimental value (GCV) in Kcal/kg	Predicted Value (GCV) by ANN in kcal/kg	Difference
1	4232.122	4057.186	174.9364
2	1905.093	1915.878	10.7848
3	3844.603	3979.216	134.613
4	4296.98	4249.424	47.556
5	5120.53	5186.986	66.4565
6	3839.435	3755.474	83.961
7	6260.741	6239.755	20.9864
8	3148.775	3189.199	40.4238
9	3429.199	3472.721	43.5222
10	5708.497	5722.977	14.4803

The model architecture has been presented in Figure 4.2. The comparison between predicted GCV by ANN model and experimental GCV has been presented in Figure 4.3.

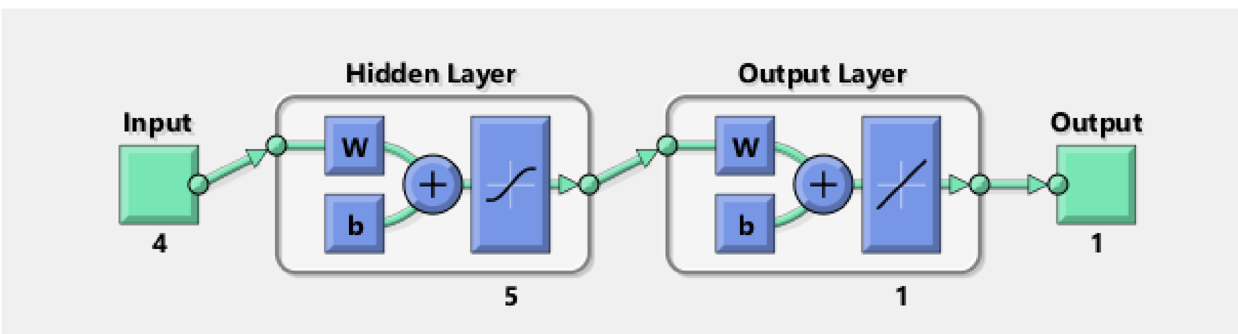

Figure 4.2: Neural Network in Model Development

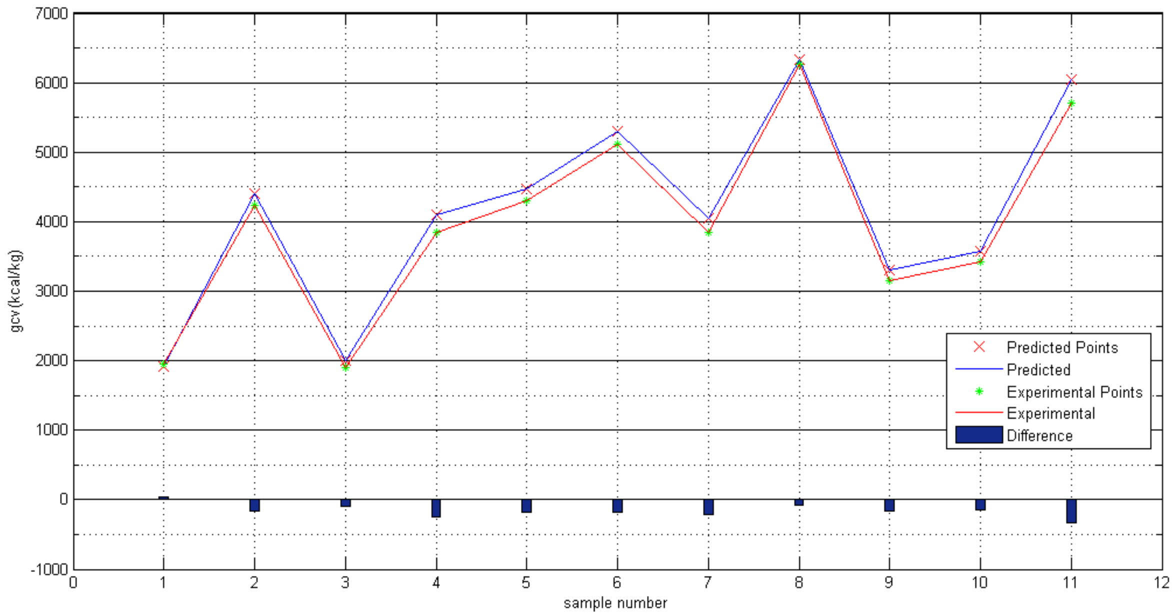

Figure 4.3: Comparison between predicted GCV by ANN model and experimental GCV

CHAPTER: 5

RESULTS AND DISCUSSION

5. DISCUSSION AND CONCLUSION

5.1 Discussion

In the present study, 59 samples were collected from different coal fields of India following the channel sampling procedure. The samples belong to South Eastern Coalfields (SECL), Singareni Collieries Company Limited (SCCL), Central Coalfields limited (CCL), Mahanadi Coalfield Ltd. (MCL), Eastern Coalfields Limited (ECL), North Eastern Coalfield Limited (NECL), Jindal Steel and Power Limited.

A study of Table 3.1 and 3.2 reveals that the moisture content of the coal samples varied from 0.6 (Sample 14) to 14.39 % (Sample 17). The volatile matter of the coal samples varied from 12.46% (Sample 51) to 43.03 (Sample 31). The fixed carbon content of the coal samples varied between 17.19% (Sample 49) to 66.35 % (Sample 14). The gross calorific values varied between 1945.34 Kcal/kg (Sample 37) and 8075.05 Kcal/kg (MCL-5). Thus it could be seen that coals that have been collected for the study covers almost all major coalfields and the quality of the coals covers a broad spectrum.

In order to understand the relationship between the calorific value and the intrinsic properties, correlation study was carried out and this has been presented in Figure 5.1 to 5.4.

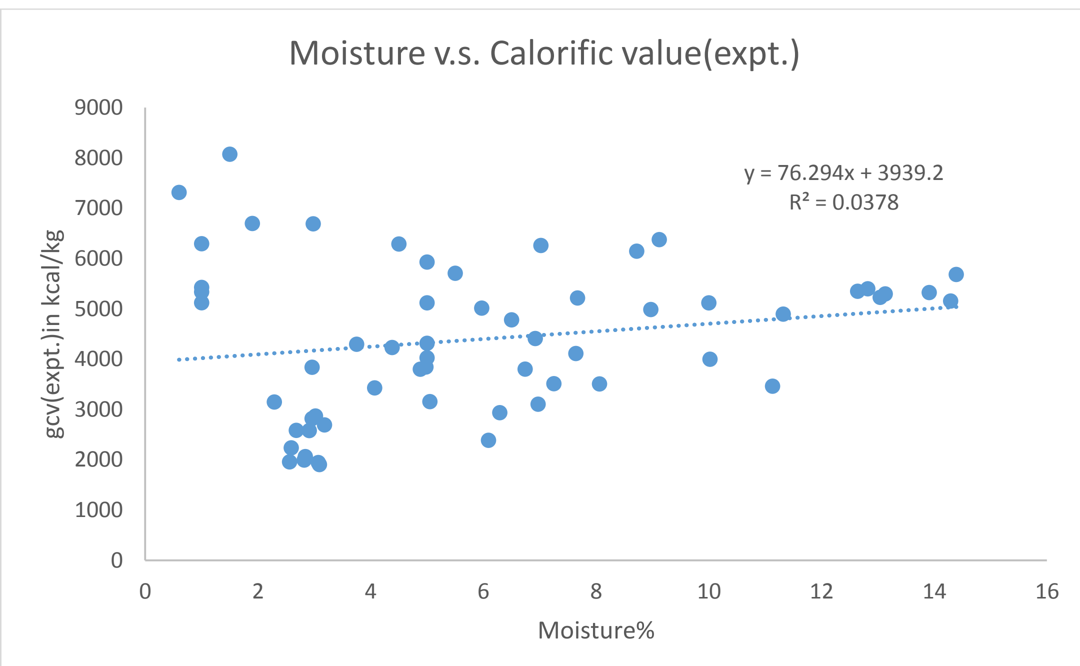

Figure 5.1: Correlation plot between moisture and experimental GCV

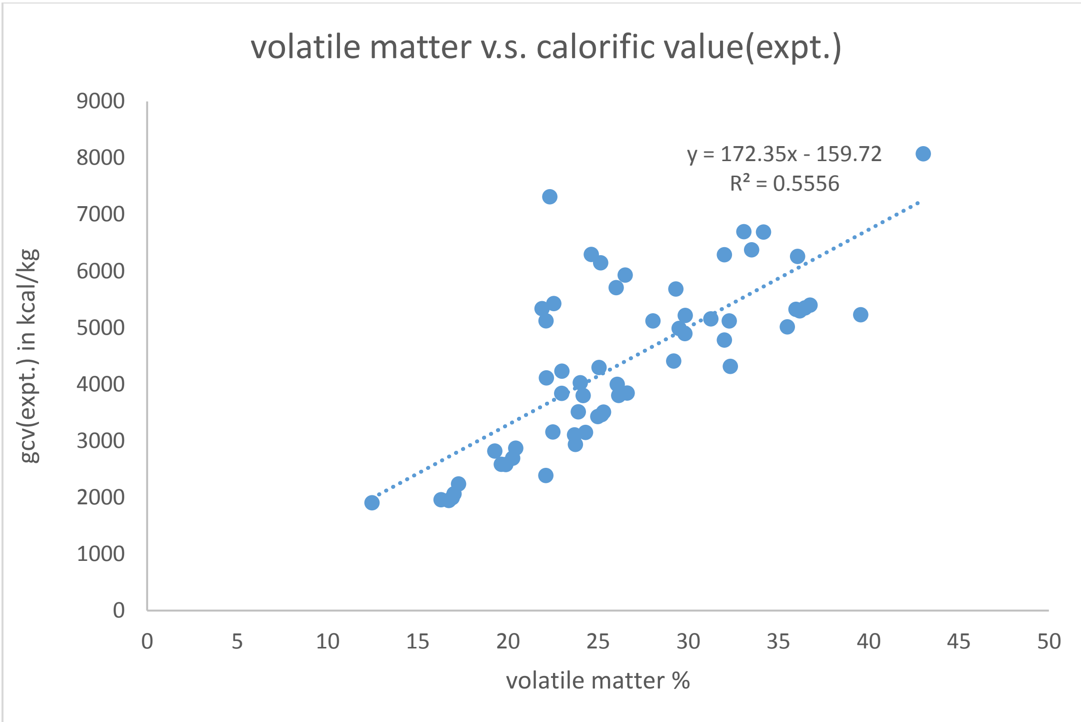

Figure 5.2: Correlation plot between volatile matter and experimental GCV

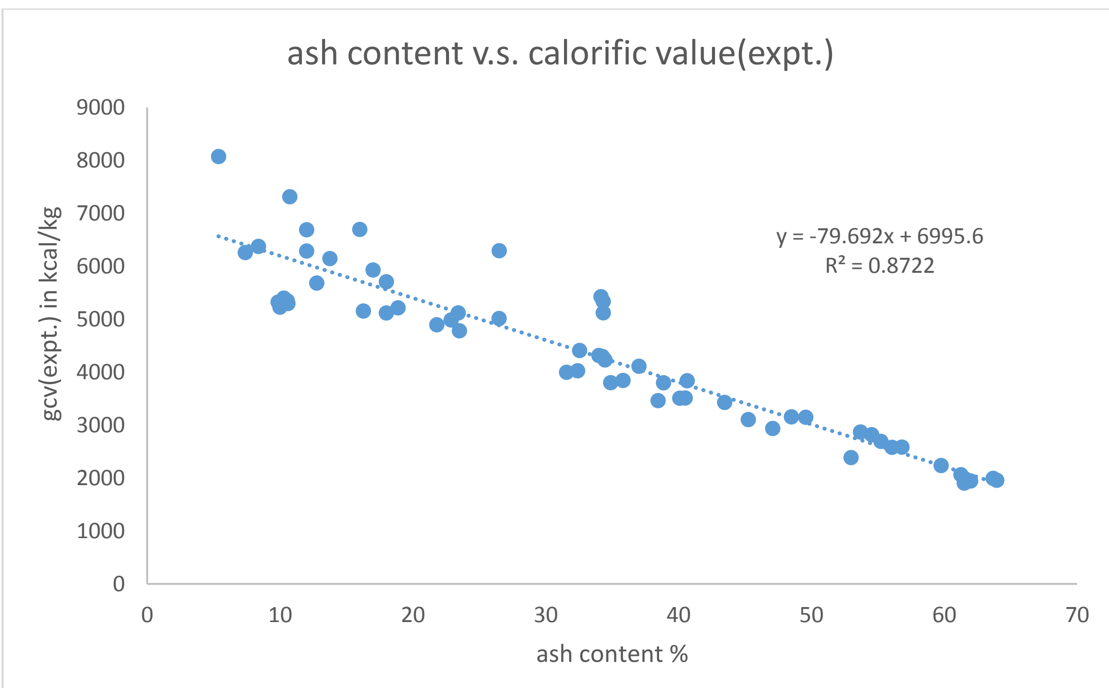

Figure 5.3: Correlation plot between Ash content and Experimental GCV

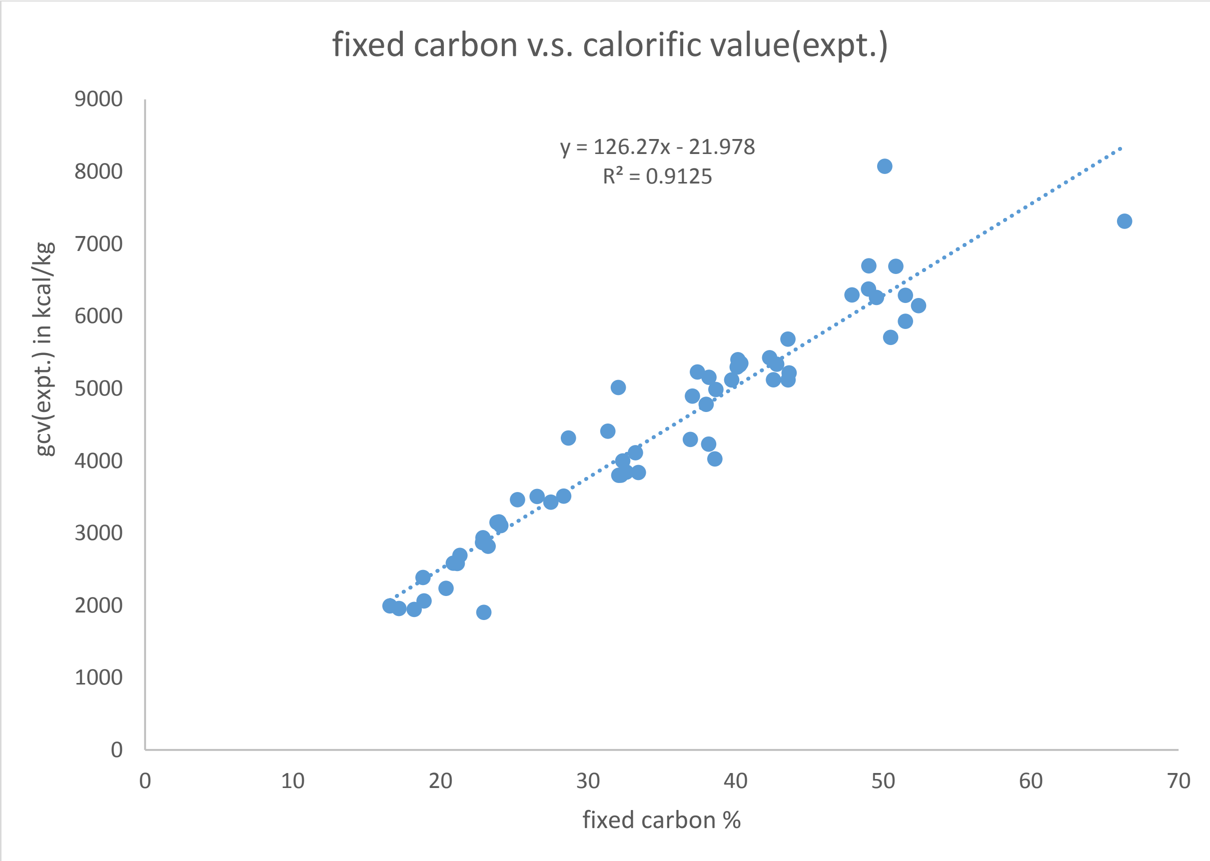

Figure 5.4: Correlation plot between fixed carbon and experimental GCV

5.1.1 Multivariable relationships of GCV with proximate analysis parameters

By regression method, the correlation coefficients of M, A and F with GCV, were determined to be -123.971,-81.312 and 20.742 respectively. Equation given by regression analysis is:

GCV = 7115.197 - 123.971*M - 81.312*A + 20.742*F $\quad$ R^2 =0.977

From above equation it can be concluded that the worthy relations are for fixed carbon with positive effect and moisture, ash with negative effect, because they are rank parameters.

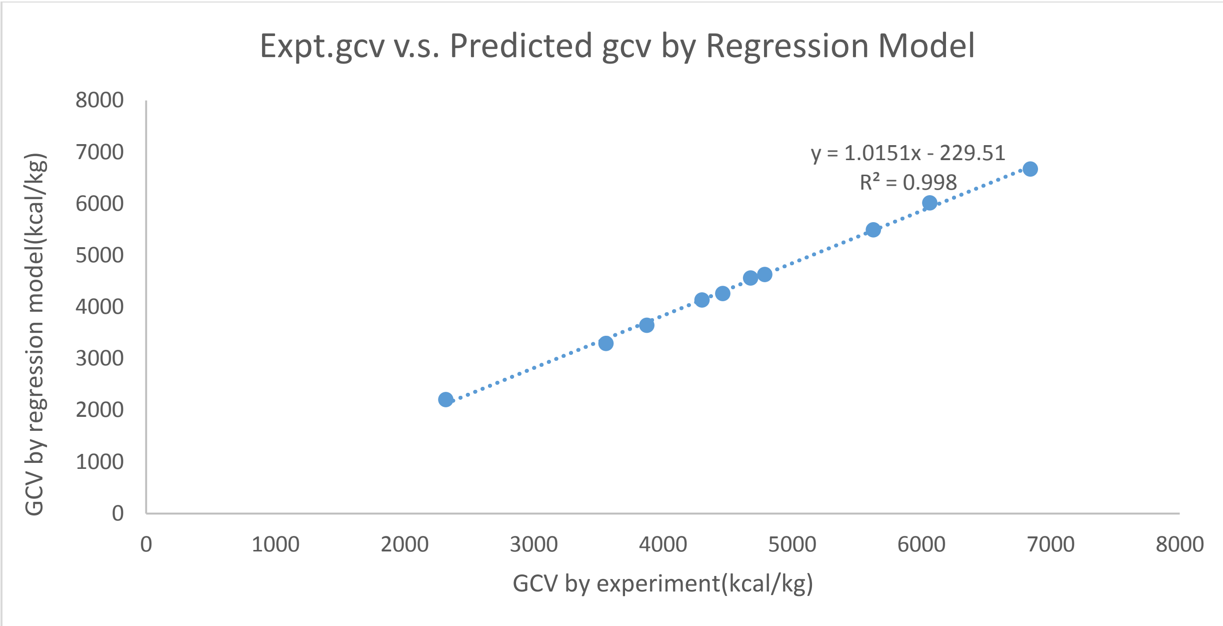

Figure 5.5: Correlation plot between Experimental GCV and GCV predicted by Regression Model

The following formulae have been developed by Central Institute of Mining and Fuel Research (CIMFR), Dhanbad for the determination of calorific value of Indians coals from their proximate analysis:

1. For low moisture coals, M <= 2%

$$C_G = 91.7\,F + 75.6\ (V - 0.1A) - 60\,M$$

2. For high moisture coals, M >= 2%

$$C_G = 85.6(100 - (1.1\,A + M)) - 60M$$

Where: M, V, A, F denote Moisture, Volatile Matter, Ash and Fixed Carbon, all in present air-dried basis, respectively.

A comparison between the predicted calorific value and the value obtained by CIMFR formulae has been presented in table 5.1

Table 5.1: Comparison of Experimental GCV and predicted GCV by CIMFR formulae

Sample no.	Experimental GCV in Kcal/kg	GCV by CIMFR formulae	Difference Kcal/Kg
1	4232.1224	4677.5184	445.396
2	1905.0932	2318.3144	413.2212
3	3844.6028	4462.1008	617.498
4	4296.98	4787.1368	490.1568
5	5120.5295	5627.7144	507.1849
6	3839.435	4301.42	461.985
7	6260.7414	6842.9872	582.258
8	3148.7752	3558.1232	409.348
9	3429.1988	3874.2728	445.074
10	5708.4967	6064.32	355.8233

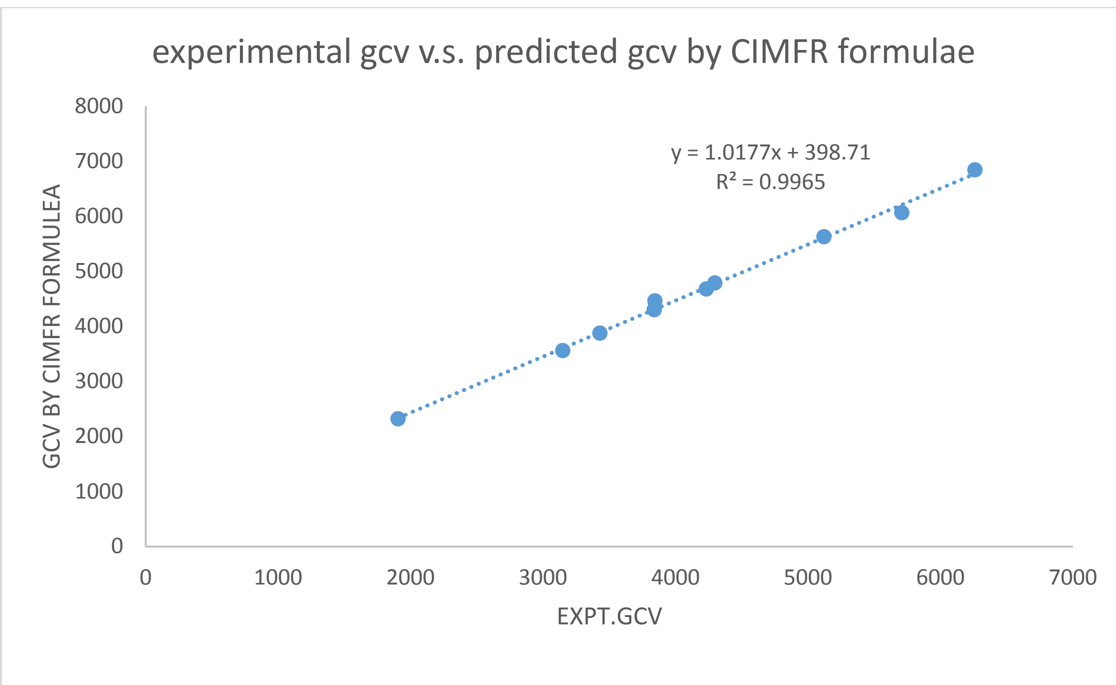

Figure 5.6: Correlation between experimental GCV and predicted GCV by CIMFR formulae

Here correlation coefficient between experimental GCV and predicted GCV by regression model and correlation coefficient between experimental GCV and predicted GCV by CIMFR formulae found to be 0.998 and 0.9965 respectively.

5.1.2 ANN-based models for GCV estimation

After the ANNs model development, predicted GCV values were compared with the experimental GCV (Figure 5.7). It was observed that correlation coefficient value of experimental GCV and predicted GCV by ANN model is 0.9954 that means it is good correlation between experimental and predicted GCV by neural network.

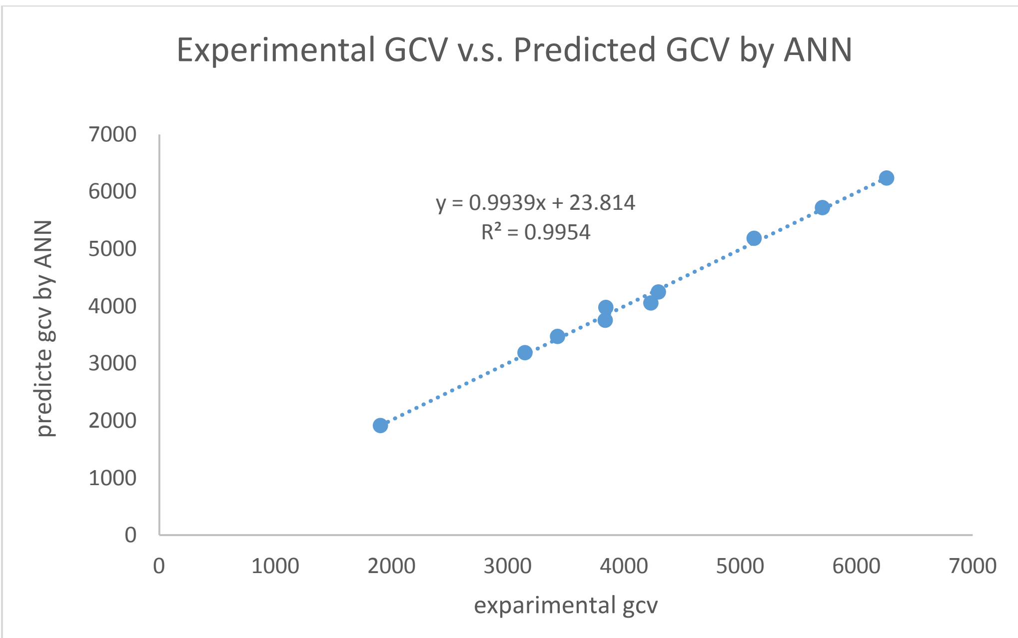

Figure 5.7 Correlation between Experimental GCV and predicted GCV by ANN

A comparison of the Gross Calorific Values (GCV) obtained by Regression Analysis, ANN model, CIMFR formulae along with the experimental value has been presented in Figure 5.8 and 5.9.

Figure: 5.8 Comparison of GCV determined from different methods using line chart

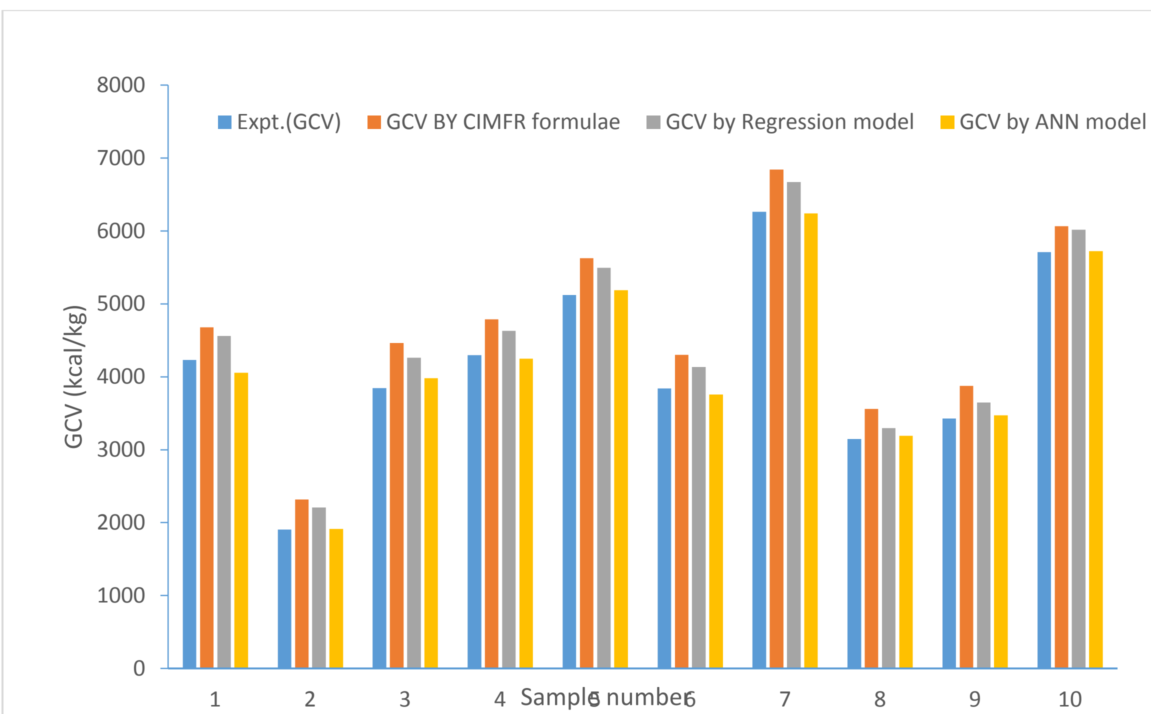

Figure: 5.8 Comparison of GCV determined by different methods using column chart

It may be observed that all the three models predict the calorific value fairly accurately. However, the ANN model gives a better prediction than the other methods. Therefore, prediction of gross calorific value by ANN model could be a viable option than experimentation in the laboratory. The ANN model considers the intrinsic properties determined by proximate analysis as input parameters, which is a routine task in the field as these are required to determine the grade of coals and hardly demand any costly experimental setup.

5.2 Conclusion

Results from the Regression and ANN analysis is show that difference between experimental and predicted is less and those models can use for prediction of GCV. Any industry where coal is utilized for heating applications, determinations of calorific value, proximate analysis and ultimate analysis are common practice to assess the quality of coals In India, due to non-availability of consistent power supply and higher industrial tariffs many industries are opting for coal-fired captive power plants. Quick assessment of coal quality by cheaper means to run the boilers efficiently is a pre-requisite, prediction of calorific value of coal based on proximate analysis data can be carried out by regression analysis and artificial neural network analysis. Regression analysis results showed that the multiple regression model is seen as the best model. The determination R^2 of the multiple regression model is 97.71%. This value is good and identifies the valid model. This result reveals the usefulness of a multiple linear regression model in the prediction of calorific value. These models are decision makers that examine coal deposit parameters, such as calorific value, ash content, and moisture content, in order to manage the coal deposit. The developed correlation involves the effects of all the major variables affecting the gross calorific value of coals. Validation with a set of data at reasonable accuracy establishes the general acceptability of the developed correlation.

By this study it was conclude that predicted GCV by Artificial Neural Network had very less difference with GCV determined by experiment. GCV predicted by ANN model also have less difference with experimental determined GCV compare to GCV predicted by other methods include regression model and CIMFR formulae. It was also found that GCV predicted by regression model have less difference with experimental determined GCV compare to GCV predicted by CIMFR formulae.

The ANN model developed for predicting calorific value of the coal gives a better prediction than the other methods. Therefore, prediction of gross calorific value by ANN model could be a viable option than experimentation in the laboratory. The ANN model considers the intrinsic properties determined by proximate analysis as input parameters, which is a routine task in the field as these are required to determine the grade of coals and hardly demand any costly experimental setup. ANN models generally require a large database for training purpose in order to improve the prediction accuracy. Once a database is generated with sufficiently large number of coal samples, it would be easier to predict the calorific value of coal accurately without determining it in the laboratory. It is expected that the results of this study will benefit the practicing mining engineers and researchers to a great extent in predicting the spontaneous heating susceptibility of the seams and accordingly plan the mining activities and precautionary measures to deal with fire problems in mines.

CHAPTER: 6

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7. REFERENCES

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