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**ML approach to study the spontaneous combustion
characteristic of coal**

Under the mentorship of Prof. Patitapaban Sahu

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DECLARATION

We hereby declare that this information is our own work to the best of our knowledge and belief, it contains no material previously or written by any other person nor material which to a sustainable extent has been accepted for the award of any degree or diploma of the university or other institute of higher learning, except where due acknowledgment and references has been made in the text.

CERTIFICATE

This is to certify that project report entitled "ML approach to study the spontaneous combustion characteristic of coal" which is being submitted by Charmila Gollavilli, Md. Athar Imam and Priyanshu Singh in partial fulfillment for the requirement for the award of the degree of the Bachelor of Technology in Department of Mining Engineering of Indian Institute of Technology (Indian School of Mines), Dhanbad, Jharkhand. They have worked under the guidance of Prof. Patitapaban Sahu (Associate Professor, Department of Mining Engineering) and have fulfilled the requirement for the submission of the project. The matter presented in this dissertation has not been submitted by me anywhere for the award of any other degree of this or any other institution. This is to certify that the above statement made by the candidate is correct and true to the best of our knowledge.

Date : 13th Nov, 2023

Prof.....
(Project Guide)

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Table of Contents

1. Introduction
2. Objective
3. Scope
4. Literature Review
5. Background
6. Methodology
7. Analysis
8. Future Work
9. References

Introduction

Coal is a very important natural resource which provides around 38.5% energy to the world. In India , coal is the most abundant fossil fuel and around 75% of the total power generation is achieved by coal. So India is highly dependent on coal for commercial energy requirements.Fires in coal mines are a major problem nowadays in the mining industry all over the world. Spontaneous combustion is a very common occurrence in coal mines and is a major factor contributing to the mine fire. It is a matter of prime concern in the mining industry. Coal found in a lot of Indian coalfields is highly susceptible to spontaneous heating. Cases of mine fires started due to spontaneous heating and continued to burn for decades are numerous, and common all over the world. An example of most spontaneous combustion susceptible coalfield is Jharia coalfield in BCCL India which has had many mine fires burning since 1925.Mine fires give rise to environmental problems, safety hazards and economic losses like air pollution,release of toxic gasses, difficult geo-mining conditions, sterilization of coal,hindrance to production, explosions, and damage to structure and properties.

Objective Of Project

To assess the spontaneous combustion susceptibility of coal using Machine learning project and correlate its intrinsic properties with susceptibility indices. The work is divided into four parts as follows:

- Sample collection and preparation according to standard procedures.
- Determination of the intrinsic properties of the collected coal samples using proximate analysis and bomb calorimetry.
- Determination of spontaneous heating susceptibilities by Crossing point temperature(CPT) test and wet oxidation potential(WOP) analysis.
- Correlation of spontaneous heating susceptibilities indices with that of the intrinsic properties.

Scope

- The project will focus on the assessment of spontaneous combustion characteristics of coal using the ML approach. The study will cover different coal samples of different mines for better assessment and training of ML models.
- Reviewing the existing literature on spontaneous combustion of coal and mining regulations and standards.

Literature Review

Erdogan KAYMAKCI and Vedat D_ IDAR_ I (2000) explore the links between coal properties and spontaneous combustion parameters. Linear regression identifies ash, volatile matter, carbon, hydrogen, exinite, inertinite, and mineral matter as key factors. Multiple regression expands this to include nitrogen, oxygen, and sulphur. The research yields empirical equations for practical application in predicting spontaneous combustion risks in coal-related industries. Overall, the study provides valuable insights into the complex relationships governing coal behaviour and combustion.

Nugroho et al. (2001) used CPT to determine the effect of particle size in case of a single type of coal on the rate of low temperature oxidation. They also studied spontaneous combustion tendencies of blended coal. It was concluded that the activation energies and reactivities of coal decreases with increasing particle size. They also found that the blended coals were more susceptible to self-heating due to higher reactivities and activation energies coupled with lower critical ambient temperatures of more reactive coals.

Pattanaik et al. (2011) collected coal samples from different coal seams of Chirimiri coalfields and did proximate analysis and differential thermal analysis .They concluded that higher ranked coals were less prone to spontaneous combustion whereas lower ranked coal were more prone to spontaneous combustion. He also found that the degree of proneness to spontaneous combustion increases with the increase of vitrinite and exinite, but decreases with the increase of inertinite content.

Choi et al. (2013) :they used CPT (Crossing Point Temperature) and gas chromatography to establish a connection between the susceptibility to spontaneous combustion and the rank of coal. The study involved three types of coal—two Indonesian Lignite and one Chinese bituminous coal. FTIR (Fourier Transform Infrared Spectroscopy) was utilised to examine the hydrocarbon composition in the coals.They concluded that coals of lower rank can react with oxygen at low temperatures making them more susceptible to spontaneous combustion than higher ranking coals.

Jun Deng et al.(2021) focuses on predicting coal spontaneous combustion (CSC) temperature using gas coal from the Zhaolou coal mine in China. They employ a simulated annealing-support vector machine (SA-SVM) model to capture the nonlinear relationship between characteristic gases and coal temperature. The model's accuracy is validated using in situ data from an actual working face, and compared to back-propagation neural network (BPNN) and single SVM methods. Results indicate that SA-SVM outperforms others in terms of prediction accuracy, robustness, error

tolerance, and environmental adaptability. The findings hold practical significance for mitigating CSC risks in coal mines and providing timely warnings.

Background

Coal mine fires

Mine fires mainly occur in coal mines but it also occurs in metal mines, for example pyrite mines. The main causes of mine fires are spontaneous combustion, blasting in mines, electrical failure and explosion of gases ,open flame,friction But spontaneous combustion is the major cause. Spontaneous combustion occurs due to self heating or self oxidation of coal when the heat produced due to oxidation is not properly dissipated

Spontaneous Combustion Theories

Spontaneous combustion may be defined as the self heating of coal or other carbonaceous

material resulting eventually in its ignition without the application of external heat or of any

oxidisable substance due to auto-oxidation.The self-oxidation of coal takes place through a series of complex physio-chemical processes which consists of events like absorption of atmospheric oxygen, formation of coal-oxygen complexes and decomposition leading to evolution of heat. The rate of oxidation at ambient environments provides an idea about the proneness of coal to auto oxidation.

For spontaneous combustion to occur, these three condition must be satisfied-

- I. Coal must be present in a form which can oxidize readily at ambient temperature.
- II. Oxygen must be available to support oxidation.
- III. Favorable conditions for accumulation of heat must be present.

The most important theories of spontaneous heating are:

1) Bacteria theory:

The bacteria present in coal can also contribute to the heat produced during self-heating. This phenomenon found in some carbon-containing materials like haystack and wood is due to this bacterial action.

However ,there is no conclusive proof to authenticate the theory. Hence it is concluded that bacteria could cause slight heating and can't be an important reason for spontaneous combustion.

2) Pyrite theory:

The pyrite present in the coal also oxidises in coming contact with air and releases large amounts of heat. It was earlier thought that the heat released on oxidation of these pyrites is the reason behind spontaneous heating of coal.



But later on researchers established that the heating due to oxidation of pyrites might aid the process of spontaneous heating but it cannot be the reason behind it as coal containing very less or no pyrites also exhibited spontaneous heating.

3) Phenol theory :

The theory suggests that within coal, phenolic hydroxyls and polyphenols exhibit quicker rates of oxidation compared to other chemical groups.

4) Coal-oxygen complex theory:

According to this theory, adsorption of oxygen takes on the surface of coal forming a less stable coal-oxygen complex at different temperatures with release of heat and oxidation products like CO, CO₂, and water.



As this reaction is exothermic, there is rise in the temperature of coal which further increases the rate of sorption of O₂ and production of heat.

Spontaneous Combustion Mechanism

When coal comes into contact with oxygen in the air, it begins to adsorb oxygen, leading to the chemical reaction resulting in the oxidation of certain constituents of coal with the production of a small quantity of heat and products such as carbon monoxide (CO), carbon dioxide (CO₂), and water vapour. Initially, these reactions occur at room temperature, and the heat generated is dissipated relatively slowly by the surrounding air.

However, if the heat is trapped due to inadequate dissipation or a slower dissipation rate compared to heat generation, it can lead to a buildup of heat. As the coal's temperature gradually increases, more portions of the coal become involved in the oxidation process, accelerating it. With further temperature rise, the reactions transition from physical processes to chemical ones. Above 70°-80°C, the previously formed peroxy-complexes begin to decompose, yielding CO, CO₂, and H₂O, causing a significant change in reaction rates and mechanisms.

As the temperature continues to rise, reaching a critical threshold, the loss of moisture leads to substantial alterations in the process. The elevated temperature promotes the formation of more stable oxygen-coal complexes. Ultimately, the temperature reaches an ignition point, causing the coal to catch fire and ignite into an open flame. Effective air circulation can help prevent the temperature from reaching critical levels.

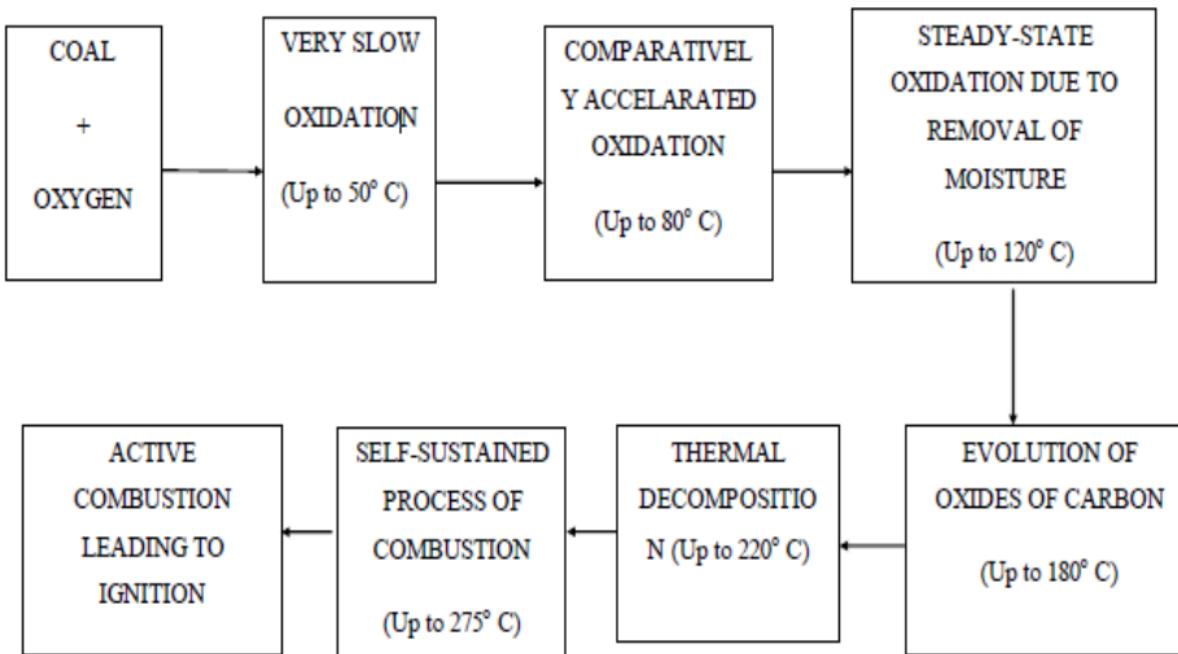


Fig- flow chart describing different stages of Spontaneous heating.

FACTORS AFFECTING SPONTANEOUS HEATING OF COAL

There are various factors which affect spontaneous combustion and each and every factor plays an important role in the process of auto-oxidation to some extent.

Some of the important factors that affect the spontaneous heating of coals are:

Intrinsic Factors (Nature of Coal)	Extrinsic factors (Atmospheric ,Geological and Mining condition)
Particle size and surface area Rank of coal petrographic contents Pyrites Moisture Ash andMineral Matters Porosity Volatile Matter	Temperature Coal Seam surrounding strata Seam Thickness Extensive development Ventilation system and Air flow rate Geological disturbance Depth of working etc.

- Surface area: The rate of oxidation of coal and hence, the amount of heat dissipated/liberated depends on the total surface area of the coal.
- Rank of coal: Lower rank generally higher in moisture , oxygen and volatile contents are more susceptible to spontaneous combustion.
- Petrographic Content: Degree of proneness to spontaneous combustion increases with the increase of vitrinite and exinite, but decreases with the increase of inertinite content.
- Volatile Matter: High volatile coals are more susceptible to spontaneous combustion.
- Moisture content: Moisture might affect coal liability to absorb oxygen by hindering its diffusion and hence its oxidation rate but Clemens et al. found that moisture could inhibit the production of stabilised radicals and quicken the oxidation of coal.
- Ash content: Ash generally inhibits the spontaneous heating of coal.
- Pyrite content: Pyrite gets easily oxidised when it comes into the contact of air. It releases high amounts of heat. So it basically contributes to spontaneous combustion.
- Temperature: Warm surroundings and air will considerably increase the oxidation rate of coal.

- Surrounding Strata: Thermal conductivity of surrounding strata play an important role in heat dissipation. If a coal heap is covered by loose shales the heat of oxidation of coal is not dissipated as fast as in the case of coverage of sand stone and the former heap is more liable to self-heating.
- Depth of working: As the depth increases temperature and crushing of strata increase which helps in accelerating spontaneous heating.
- Seam Thickness: As the percentage of extraction of coal is not 100% in any method. So there are high losses of coal while extraction. These left coal are responsible for spontaneous combustion.
- Geological disturbances: Near the geological disturbance like faults the coal is in the crushed state. Such crushed coal is more prone to spontaneous heating.
- Method of Working : method of working also the spontaneous combustion of coal. The Board and Pillar method is more prone to spontaneous heating than the Longwall Mining method.
- Ventilation system and air flow rate: Leakage of air in closed panels may lead to self heating. An adequate air velocity is required to proper dissipation of heat from the UG mine. Faulty ventilation systems and improper velocity of air will also cause self heating .

Methodology

To identify the characteristics of coal and study the effects of various parameters of coal that affect its combustion and spontaneous heating tendency of coal, the following experiments are needed to be carried out

- Proximal Analysis
- Wet Oxidation Potential
- Crossing Point Temperature

Sample Collection

Sampling is the process of collection of a small portion of a whole for experimental purposes so that the small portion represents the properties of the whole substance. It is a critical step in assessing the quality and characteristics of a coal deposit or shipment. The goal of sampling is to obtain a sample that accurately reflects the overall composition and properties of the entire coal lot, ensuring that subsequent analyses are representative of the entire quantity. The collected samples are sent to a laboratory for

various analyses, including proximate analysis, ultimate analysis, calorific value determination, and other tests to assess the coal's quality and properties.

Various types of sampling are:

1. Chip sampling
2. Channel sampling
3. Drill-hole sampling
4. Bulk sampling

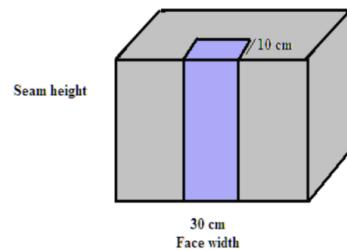


Fig. chip sampling

For the fulfillment of the experiment, the commonly adopted channel sampling method is carried out. Channel sampling provides a more systematic and controlled way of collecting representative samples compared to methods like chip sampling.

Channel Sampling

A channel or groove is cut into the exposed rock using tools such as a rock saw or chisel. Samples are collected from the channel floor and walls, capturing a cross-section of the rock. The width of the channel is typically a few centimeters to capture a representative cross-section of the rock. Common widths range from 5 centimeters (2 inches) to 15 centimeters (6 inches) and around 8-10 cm in depth. Sample intervals are set at a specified width, usually ranging from 1 to 20 feet, commonly 5 feet. This allows for a representative sample to be acquired as the sample is not biased.

Coal Sample Preparation:

The samples obtained from the mines by channel sampling are crushed in the laboratory as per the experimental requirements. The crushed samples are then sieved to required sizes and stored in airtight polythene zippers. The packets are stored in air tight containers for further use in experimentation. They are carefully stored as per their sizes and marked with labels on the containers to differentiate easily. And then the proximate analyses of the coal samples will be observed.

Determination of Intrinsic properties of Coal :

Proximate Analysis

One of the methods for Proximate analysis is one of the first analyses performed on coal after mining. The test involves heating the coal under various conditions for variable amounts of time to determine i) moisture content ii) volatile matter iii) fixed carbon and vi) ash yield.

The apparatus required for proximate analysis is a muffle furnace of good temperature control, an analytical balance of good sensitivity (± 0.1 mg), a crucible made up of aluminium or silica, and an oven with good temperature control (± 3 °C), and a desiccator.



Fig. Hot Air Oven for proximate analysis

Determination of Moisture Content (M)

This is defined as the percentage of moisture in a sample under examination when it is heated just over the boiling point of water (105°C). The heat given at this temperature evaporates the water from the sample of the coal, which changes the original weight of the coal. At the point that it stops changing, the difference between the initial weight and the final weight expresses the moisture content that is the weight loss. It is expressed as a percentage of coal material.

Procedure:

- About 1g of air-dried coal sample is finely powdered and weighed in a silica crucible.
- It is then placed inside an electric hot air oven without a lid which is maintained at 105°C - 110°C and allowed to remain there for 1 hour.
- It was then taken out with a pair of tongues, and cooled in desiccators for about 15 minutes and then weighed. Desiccators consist of unhydrous Calcium chloride which absorbs moisture that can be absorbed during cooling.
- The loss in weight is observed as moisture percentage.

Moisture percentage is calculated as per the following formula.

- % of Moisture = (Loss in weight of coal sample / weight of coal taken) X 100
i.e,

$$\text{Moisture\%} = (W_2 - W_3 / W_2 - W_1) \times 100$$

W_1 = weight of empty crucible, g

W_2 = weight of crucible and coal sample before heating, g

W_3 = weight of crucible and coal sample after heating, g

Determination of Volatile Matter (VM)

Volatile matter consists of the gases and vapours released from the coal when it is heated in the absence of air. This includes substances like hydrocarbons, hydrogen, carbon monoxide, methane, and other volatile organic compounds. The measurement of volatile matter is crucial because it influences combustion behaviour and energy content. Volatile matter is defined as the gases driven off when coal is heated to 950°C (1742°F) in the absence of air under specified conditions. Volatile matter is measured practically by determining the loss of weight. Volatile matter decreases as rank increases.

Procedure

- First the empty volatile matter crucible is weighed.
- The 1g of coal sample is weighted in the Crucible and it is covered with a lid and placed in a muffle furnace maintained at $925\pm20^{\circ}\text{C}$ for exactly 7 minutes. With a lid because we want to lose only the toxic gasses and not the other content of the coal.
- After that it is taken out of the muffle furnace and kept out for cooling in open air, then in a desiccator and weighted again.
- To calculate the volatile matter following formula is used
$$\% \text{ Volatile matter} = (\text{loss in weight at } 925^{\circ}\text{C}/ \text{weight of coal taken}) \times 100$$
i.e,
$$\% \text{ Volatile matter} = (W_2 - W_3/W_2 - W_1) \times 100$$
where, W_1 = weight of empty crucible, g
 W_2 = weight of crucible and coal sample before heating, g
 W_3 = weight of crucible and coal sample after heating, g

Determination of Ash Content (A)

Ash is the inorganic residue that remains after combustion. It is the impurities consisting of inorganic matter from the earth's crust like limestone, iron, aluminium, clay, silica, and trace elements. It is the incombustible material remaining after combustion of coal. The measurement of ash content is essential for assessing the mineral composition and potential environmental impacts during combustion. The ash content of pulverised coal lowers the carbon content and calorific value of the coal injected and requires additional fluxes to remove this material as slag, both of which affect the heat balance of the blast furnace, potentially leading to an increase in fuel rate and a decrease in productivity. Understanding the intrinsic properties of ash content is essential for assessing the quality and suitability of coal for various applications.

Procedure:

- The residual coal in the crucible is then heated without a lid in that muffle furnace at $700\pm50^{\circ}\text{C}$ for half an hour.

- After heating, cool the crucible in a desiccator to prevent moisture absorption.
- Weigh the crucible with the remaining ash.
- The difference in weight before and after heating represents the ash content.
- To calculate the Ash content following is the formula:
- % Ash = (weight of residual left in crucible /weight of coal taken)X100
i.e,

$$\% \text{ Ash content} = (W_3 - W_1 / W_2 - W_1) \times 100$$

where, W_1 = weight of empty crucible, g
 W_2 = weight of crucible and coal sample before heating, g
 W_3 = weight of crucible and coal sample after heating, g

Determination of Fixed Carbon (FC)

Fixed carbon is the carbon found in the material which is left after volatile materials are driven off. It primarily consists of carbon and, to a lesser extent, inorganic minerals. Fixed carbon is an indicator of the carbon content available for combustion and is a major contributor to the heating value of coal. It is determined by the difference between 100 and the sum of the percentages of volatile matter, ash, and moisture.

$$\% \text{ of Fixed Carbon} = 100 - (\% \text{ of Total Moisture} + \% \text{ of Volatile Matter} + \% \text{ of Ash content})$$

Determination of susceptibility of coal to spontaneous combustion :

- Wet oxidation potential
- Crossing Point Temperature

Wet oxidation potential (WOP):

Wet oxidation potential (WOP) of coal is one of the most relied indices used for assessing the spontaneous combustion susceptibility of coal. During spontaneous combustion modelling and simulation, volatile matter can be used as the most influential parameter for assessing the fire risk of the coal samples considered in the study. Further, the partial dependence analysis was done to interpret the complex relationships between the WOP and intrinsic properties of coal. In the wet oxidation potential method emphasis is given to change in potential difference during the oxidation process. It has been investigated that 0.2N KMnO₄ with 1N KOH solution is the optimum mixture to carry out wet oxidation potential method for obtaining best response to spontaneous heating of coal.

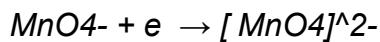


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Principle of Wet Oxidation Potential:

The principle of wet oxidation potential involves assessing the reactivity of coal towards spontaneous combustion by measuring changes in electrode potential during the oxidation of coal in the presence of an alkaline potassium permanganate (KMnO_4) solution. The reduction of permanganate ion (MnO_4^-) to manganate ion (MnO_4^{2-}) serves as the indicator for the oxidation process. The standard electrode potential (E_0) for this redox reaction is 0.56V.



The electrode potential (E) during the wet oxidation potential experiment can be calculated using the Nernst equation:

$$E = E_0 - (RT/F) \ln ([\text{MnO}_4]^{2-} / [\text{MnO}_4^-])$$

Where,

E = electrode potential

E_0 =standard electrode potential (0.56 V for the given redox reaction),

R = Universaltgastconstant

T = Temperature

F = Faraday's Constant

The wet oxidation potential experiment monitors changes in electrode potential during the oxidation of coal in the presence of potassium permanganate.

Apparatus required :

Beaker, Saturated calomel electrode (Hg/Hg₂Cl₂/KCl), Carbon electrode , Millivoltmeter, Magnetic stirrer with a Teflon-coated fish and Calibrated temperature recorder.

Coal Sample Preparation:

0.5g of a -212- μ m sized coal sample added to the chemical mixture.

Experimental Setup:

- A beaker is used as the reaction vessel for the wet oxidation process. It contains a chemical mixture comprising potassium permanganate ($KMnO_4$) as the oxidizer in potassium hydroxide (KOH) solution.
- A Teflon-coated fish of the magnetic stirrer is placed inside the beaker to ensure continuous stirring of the solution.
- The temperature of the mixture is measured using a calibrated temperature recorder. The temperature recorder helps monitor the temperature changes during the oxidation process.
- A 0.2 N solution of potassium permanganate ($KMnO_4$) is prepared in 1 N KOH solution. This mixture serves as the oxidizer for the wet oxidation process.

Procedure:

- The beaker, along with electrodes and the chemical solution of 100 ml of deci-normal potassium permanganate ($KMnO_4$) in 1N potassium hydroxide (KOH) solution, is placed over a magnetic stirrer such that such that homogeneity of the mixture of coal and alkali solution is maintained.
- A calomel reference electrode and a carbon electrode are immersed in the $KMnO_4$ -KOH solution.
- The potential difference (EMF) in millivolts (mV) is measured between these electrodes using a millivoltmeter after attaining a stable reading.
- The Teflon coated fish of the magnetic stirrer is placed inside the beaker.
- 0.5 g of coal sample with a particle size of -212 microns is added to the mixture.
- The mixture is continuously stirred using a Teflon coated fish of the magnetic stirrer.
- The potential difference (EMF) was recorded between the calomel and carbon electrodes over a period of time by using a millivolt metre till the potential difference attained a nearly constant value.
- Temperature and potential difference readings are recorded at 1 minute intervals.
- Experiments are carried out at 45°C.

Calculation and analysis :

- The difference between the potential difference (PD) of the mixture before adding the coal sample and after complete oxidation of the coal sample is calculated for each sample.
- Record the total time taken for each experiment to calculate the rate of reduction of potential difference (RPD), expressed in millivolts per minute

- This parameter is considered as the susceptibility index of coal towards spontaneous combustion and is expressed in mV.

Objectives and Significance:

This method provides a means to quantitatively evaluate the likelihood of coal self-heating and spontaneous combustion, offering crucial insights into the reactivity and combustion characteristics of coal samples. Understanding these parameters aids in designing safety measures and preventive strategies in coal handling and storage, particularly in scenarios where spontaneous combustion is a concern.

Crossing Point Temperature (CPT)

Crossing Point Temperature : Crossing point temperature (CPT) is the temperature at which the coal temperature coincides with that of the furnace temperature or bath temperature in °C. CPT or critical oxidation temperature gives an idea about the proneness of coal to auto oxidation or self-heating. This is a standard method followed in India for finding out the susceptibility of coal to spontaneous combustion. The higher the crossing point temperature value, the less will be the susceptibility of coal to spontaneous heating.

Experimental setup:

The following is the setup for determining crossing point temperature of coal:

- A vertical tubular furnace having heating capacity of 3kw.
- The furnace is provided with a temperature controller and digital screen.
- The reaction tube is of glass having 26 mm internal diameter and 150 mm in length.
- The reaction tube is surrounded by a spiraling glass tube of 6 mm internal diameter which is connected to the bottom of the reaction tube for air inlet and a small outlet tube at the top acts as air/gas outlet.
- Flow meter and pressure flow control valves.
- Potassium hydroxide is used to remove carbon dioxide in the incoming air.
- Concentrated sulphuric acid to remove moisture in air.
- Drying tower containing granular calcium chlorides to remove moisture from air.

Procedure: In this method coal samples are heated in an oxidizing atmosphere in a furnace within a reaction tube at a constant rising temperature in which oxygen/air is passed at a constant flow rate of 80 ml/min through a bed of coal powder immersed in a glycerin bath heated to raise the temperature at a constant rate. Initially, the temperature of the coal bed shows a lower value than the bath temperature. As the oxidation of coal is an exothermic reaction, it evolves heat and the temperature of the

coal bed increases gradually. The oxidation rate is enhanced, and a time comes when the temperature of the coal bed equals that of bath temperature and then exceeds it. The point at which coal bed temperature equals the glycerin bath temperature is called the crossing point temperature or critical oxidation temperature of the coal concerned.

The following steps are

1. 20 gm of coal sample of size -212 micron is placed in the reaction tube where glass wool is followed at the bottom most part of the glycerin bath.
2. The tube is then lightly tapped with the help of cork a fixed number of times to achieve uniform packing density of the samples.
3. Then the reaction tube is placed in the tubular furnace, and a thermocouple is inserted at the center of the sample for the CPT experiment.
4. After switching on, the furnace air is allowed to pass through the sample simultaneously with an average heating rate of 1°C/min, and airflow is 80 ml/ min.
5. The furnace and the coal sample temperatures are recorded at every five-minute interval until their temperatures are equal or till the temperature of coal crossed over and went beyond the furnace temperature.



Fig - Reaction tube



Fig- CPT apparatus

Table : Scale to determine proneness of coal towards spontaneous heating

CPT , °C	Spontaneous combustion susceptibility
120-140	Highly susceptible
140-160	Moderately susceptible
>160	Poorly susceptible

Parameters Affecting Spontaneous Combustion

- Ash (%): Higher ash content generally reduces the likelihood of spontaneous combustion.
- Carbon (%): A higher carbon content might contribute to increased combustion potential.
- Calorie (%): The calorie content indicates the energy available; higher values might contribute to combustion.
- Exinite (%): The presence or absence of exinite can affect the susceptibility to spontaneous combustion.
- Fixed Carbon: Higher fixed carbon content might increase the tendency for spontaneous combustion.
- Hydrogen (%): Hydrogen content can influence the combustion characteristics of coal.
- Inertinite (%): The presence of inertinite may impact the coal's susceptibility to spontaneous combustion.
- Moisture (%): Changes in moisture content can affect the likelihood of spontaneous combustion; lower moisture is generally favorable.
- Mineral Matter (%): Higher mineral matter might reduce the potential for spontaneous combustion.
- Nitrogen (%): Nitrogen content can influence combustion characteristics.
- Oxygen (%): Oxygen content may affect the coal's combustibility.
- Sulphur (%): Higher sulphur content might contribute to spontaneous combustion.
- Vitrinite (%): Vitrinite content can impact the coal's combustion properties.
- Volatile Matter (%): Higher volatile matter content generally increases the tendency for spontaneous combustion.
- Pyrite content accelerates spontaneous combustion.
- Changes in moisture content influence coal's susceptibility to spontaneous heating.
- Decreasing particle size and increasing exposed surface area enhance the tendency for spontaneous combustion.
- Lower rank coals exhibit higher susceptibility to spontaneous combustion.
- Ash content generally reduces the likelihood of spontaneous heating, but specific components like lime, soda, and iron can accelerate it.
- Oil shale bands adjacent to coal seams play a role in mine fires.
- Underground atmosphere temperature directly impacts spontaneous combustion.
- Presence of faults and zones of weakness contributes by allowing air leakage, promoting combustion.

- Partial extraction mining methods, leaving part of the coal seam, can contribute to spontaneous combustion.
- Air flow rate complexities, including critical quantities, influence coal oxidation and heat accumulation.
- High ventilation differentials and changes in the mine ventilation system affect the development of spontaneous combustion.

Parameter used for Machine Learning Model

<ul style="list-style-type: none"> ● Moisture (%wt) ● Ash (%wt) ● Volatile Matter (%wt) ● Fixed Carbon (%wt) ● C (%wt) ● H (%wt) 	<ul style="list-style-type: none"> ● N (%wt) ● S (%wt) ● O (%wt) ● Calorific Value (MJ/kg) ● Vitrinite Reflectance (VRm)
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Analysis

Model Performance

Training Metrics:

- Training R-squared (R^2): A measure of how well the model explains the variability in the training data. A value of 0.96 indicates a very good fit.
- Training Explained Variation: This is another measure of how well the model explains the variation in the training data. A value of 0.96 suggests that 96% of the total variation in the training data is explained by the model.
- Training MAPE (Mean Absolute Percentage Error): An average of the absolute percentage errors between predicted and actual values. A lower value (1.38) indicates good accuracy in predictions.
- Training Mean Squared Error (MSE): Measures the average squared difference between predicted and actual values. A value of 6.83 indicates relatively low error.
- Training RMSE (Root Mean Squared Error): The square root of the MSE, providing a measure of the spread of errors. A value of 2.61 is relatively low.
- Training MAE (Mean Absolute Error): Measures the average absolute difference between predicted and actual values. A value of 2.15 indicates relatively low error.

Test Metrics:

- Test R-squared (R^2): The model's performance on new, unseen data. A value of 0.6 suggests a decent fit, but it's lower than the training R-squared, indicating potential overfitting or a need for model improvement.

- Test Explained Variation: Similar to training explained variation, it indicates how well the model explains the variation in the test data. A value of 0.65 suggests moderate performance.
- Test MAPE (Mean Absolute Percentage Error): An average of the absolute percentage errors in the test set. A value of 3.0 indicates a reasonable level of accuracy but is higher than the training MAPE.
- Test Mean Squared Error (MSE): Measures the average squared difference between predicted and actual values for the test set. A value of 22.95 suggests higher error compared to the training set.
- Test RMSE (Root Mean Squared Error): The square root of the MSE for the test set. A value of 4.79 indicates a larger spread of errors compared to the training set.
- Test MAE (Mean Absolute Error): Measures the average absolute difference between predicted and actual values for the test set. A value of 4.67 suggests higher error compared to the training set.

The relationships between the various parameters and CPT based on the correlation coefficients:

Moisture (%wt) (-0.573389):

- There is a moderate negative correlation. As CPT increases, meaning as the coal petrographic type tends toward higher values, the moisture content tends to decrease. This suggests that higher CPT is associated with drier coal.

Ash (%wt) (0.858422):

- There is a strong positive correlation. As CPT increases, the ash content tends to increase. This indicates that higher CPT is associated with a higher percentage of ash in the coal.

Volatile Matter (%wt) (-0.786662):

- There is a strong negative correlation. As CPT increases, the volatile matter content tends to decrease. This suggests that higher CPT is associated with a lower proportion of volatile matter in the coal.

Fixed Carbon (%wt) (-0.508821):

- There is a moderate negative correlation. As CPT increases, the fixed carbon content tends to decrease. Higher CPT is associated with a lower percentage of fixed carbon in the coal.

C (%wt) (0.796311):

- There is a strong positive correlation. As CPT increases, the carbon content tends to increase. This implies that higher CPT is associated with a higher percentage of carbon in the coal.

H (%wt) (-0.188262):

- There is a weak negative correlation. As CPT increases, the hydrogen content tends to decrease slightly. The correlation is not very strong, indicating that the relationship between hydrogen content and CPT is not as clear.

N (%wt) (0.689006):

- There is a strong positive correlation. As CPT increases, the nitrogen content tends to increase. This suggests that higher CPT is associated with a higher percentage of nitrogen in the coal.

S (%wt) (0.116308):

- There is a weak positive correlation. As CPT increases, the sulphur content tends to increase slightly. The correlation is not very strong, indicating that the relationship between sulphur content and CPT is not pronounced.

O (%wt) (-0.771717):

- There is a strong negative correlation. As CPT increases, the oxygen content tends to decrease. Higher CPT is associated with a lower percentage of oxygen in the coal.

Calorific Value (MJ/kg) (-0.805671):

- There is a strong negative correlation. As CPT increases, the calorific value tends to decrease. This indicates that higher CPT is associated with coal of lower calorific value.

Vitrinite Reflectance (VRm) (0.689290):

- There is a strong positive correlation. As CPT increases, the vitrinite reflectance tends to increase. This suggests that higher CPT is associated with a higher degree of vitrinite reflectance.

Future Work

Coal Mine Exploration:

- Conduct visits to various coal mines for comprehensive exploration.
- Collect diverse coal samples representing different geological conditions.

Proximate Analysis and CPT Measurement:

- Perform proximate analysis on collected coal samples to determine key properties.

Ultimate Analysis of Coal Samples:

- Conduct a thorough ultimate analysis on the coal samples to identify the elemental composition.
- Gain insights into the quality and potential applications of the coal based on its ultimate composition

Machine Learning Model Training with Real Data:

- Train sophisticated models using authentic data acquired from coal mines.
- Ensure the models are well-equipped to handle real-world variations and complexities.

Machine Learning Model Comparison:

- Implement various machine learning models to assess and compare their performance.
- Evaluate the efficacy of each model in predicting coal-related parameters.

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