Arab J Geosci
DOI 10.1007/s12517-015-2095-x

ORIGINAL PAPER

Standardization of a method for studying susceptibility of Indian coals to self-heating

Haider Banka[1] · **Santosh Kr. Ray**[2] · **D. C. Panigrahi**[3]

Received: 2 December 2014 / Accepted: 10 September 2015
© Saudi Society for Geosciences 2016

Abstract This paper establishes the standardization of an electro-chemical method called wet oxidation potential (WOP) technique for determining the susceptibility of coal to spontaneous combustion. A total of 78 coal samples collected from 13 different mining companies, spread over most of the Indian Coalfields, have been used for this investigation. Experiments were carried out at different concentrations of $KMnO_4$, viz., 0.05, 0.1, 0.15, and 0.2 N in 1 N KOH and at 27, 40, and 45 °C. With a combination of different concentrations of $KMnO_4$ and temperature, 12 experiments were carried out for each coal sample. Altogether, 936 experiments have been carried out by adopting different experimental conditions to standardize WOP method for wider applications in mining industries. Physical, chemical, and petrographical compositions of coal samples were studied by proximate, ultimate, and petrographic analyses. In order to determine the best combinations of experimental conditions to achieve optimum results in wet oxidation potential method, results were first analyzed by principal component analysis and then by artificial neural network analysis. These analyses clearly reveal that susceptibility index "rate of reduction of potential difference" (RPD12), keeping experimental condition with 0.2 N $KMnO_4$ in 1 N KOH solution at 45 °C, produces optimal results in finding out the susceptibility of coal to spontaneous heating. Further, coals are classified according to their proneness to spontaneous heating with multilayer perceptron (MLP) classifier. A correct classification with accuracy of 94.29 % on test data has been achieved with this classifier. The results have been further validated by tenfold cross-validation method to show its consistent performance over the chosen features.

Keywords Spontaneous heating · Wet oxidation potential · Principal components analysis · Artificial neural network · MLP classifier · Tenfold cross validation

Introduction

Coal mine fire, a major problem worldwide, is caused primarily by spontaneous combustion. Spontaneous combustion is defined as the slow, low-temperature flameless form of combustion sustained by the heat evolved when oxygen directly attacks the surface of a condensed-phase fuel (Ohlemiller 2002). Self-heating would be facilitated in conditions where large mass of coal is involved and ventilation is neither too little to restrict coal–oxygen interaction nor too high to dissipate away all the heat generated from above (Banerjee 2000).

The increasing international trade, in both metallurgical and steam coal, has led to renewed interest in the potential for spontaneous combustion occurring during transportation, particularly by bulk carriers. Coal stockpiles are prone to smouldering combustion especially where large quantities are stored for a long span of time. It revealed from the analysis of occurrence of these fires that most of them could have been averted if suitable preventive measures had been taken. The first step for taking such measures is to assess the susceptibility of coal seams. Attempts have been made to determine the self-heating tendency of coal based on their constituents

✉ Santosh Kr. Ray
santoshray8@gmail.com

[1] Department of Computer Science and Engineering, Indian School of Mines, Dhanbad 826004, India

[2] CSIR-Central Institute of Mining and Fuel Research, Dhanbad 826015, India

[3] Department of Mining Engineering, Indian School of Mines, Dhanbad 826004, India

Published online: 22 February 2016

obtained from proximate and ultimate analyses. Gradations are made particularly by using inherent moisture content, volatile matter content, and oxygen percentage. A study of coal and oxygen interaction clearly reveals that the process of spontaneous combustion is governed by a number of factors which may be broadly categorized as intrinsic and extrinsic parameters. Intrinsic parameters are associated with nature of coal, which are defined, either by its physical characteristics, viz., moisture, ash, volatile matter, and fixed carbon, or chemical characteristics, viz., carbon, hydrogen, nitrogen, sulphur, or petrographic distribution like vitrinite, inertinite, liptinite, and mineral matter content. Extrinsic parameters are mainly site specific and are related to geological conditions, mining methods, and environmental conditions prevailing during the extraction of coal. Many researchers have tried to correlate the spontaneous heating susceptibility of coal with the intrinsic properties (Didari 1988; Ghosh 1986; Panigrahi et al. 2000; Kaymakci and Didari 2002; Beamish and Arisoy 2008a; Beamish and Arisoy 2008b). Peroxy complex formation of coal during oxidation has also been used to evaluate its spontaneous combustion susceptibility (Behera and Mohanty 2009; Banerjee et al. 1988). Ozdeniz (2010) determined spontaneous combustion in an industrial-scale coal stockpile. Baris et al. (2012) investigated low-temperature oxidation of four different-rank Turkish coals experimented at 40, 60, and 90 °C in order to assess the effects of temperature, particle size, coal petrography, and coal rank by monitoring CO_2 and CO formation rates and calculated CO/CO_2 ratios. Carras et al. (2009) measured greenhouse gas (CO_2 and CH_4) emissions from spoil piles, coal rejects, and tailings due to low-temperature oxidation and spontaneous combustion at open cut coal mines in Australia. Lang and Fu-Bao (2010) of PR China made a comprehensive hazard evaluation system for spontaneous combustion of coal in underground mining. Xuyao et al. (2011) determined crossing point temperature of 11 coal samples of varied rank collected from different coalfields using self-designed experimental system.

In India, susceptibility of coal to spontaneous combustion is determined by using crossing point temperature method. It has been observed by earlier researcher (Banerjee 2000) that in the case of high moisture coals usually having high susceptibility, there is a shift of the crossing point temperature to a high value, because of release of moisture during heating, indicating that the coal is poorly susceptible, but in reality, it is a highly reactive coal. Therefore, some researchers advocate that susceptibility of a particular coal should be determined by different methods to ascertain its liability fairly accurately. This idea did not gain its ground as some of methods require elaborate and costly experimental setups.

Keeping this in view, wet oxidation potential method, a simple experimental technique, has been tried in the present investigation. It is evident from the review of literature that wet oxidation potential (WOP) technique has been applied to a very few samples and on a limited scale by only two researchers. Tarafdar and Guha (1989) conducted wet oxidation experiments with seven coal samples and observed that the higher the potential difference, the more susceptible the coal toward smouldering combustion. Panigrahi et al. (2004) conducted experiments with 12 coal samples from Indian coalfields. As indicated by these researchers, WOP method is one of the promising methods which should be investigated in a wider scale. Keeping these points in mind, the present investigation aims to study this method extensively over a wide range of samples with variation in concentration of oxidants and standardize it for wider application, so that it can be used by the practicing mining engineers for determining the susceptibility of coal to spontaneous heating.

Physical, chemical, and petrographical compositions of coals were studied by proximate, ultimate, and petrographic analyses. In order to determine the best combinations of experimental conditions to achieve optimum results in wet oxidation potential method, results are first analyzed by principal components analysis and then by artificial neural network analysis.

Principal component analysis (PCA) is a well-established technique for dimensionality reduction and multivariate analysis. Examples of its applications include data compression, image processing, visualization, exploratory data analysis, pattern recognition, modeling of rock fragmentation, prediction of ventilation methane emission rates in longwall mines, and time series prediction (Esmaeili et al. 2014, Labib and Vemuri 2004, Karacan 2008). In order to find out the effective parameters responsible for susceptibility of coal to spontaneous heating, the PCA technique was applied in this study.

Artificial neural network (ANN) has been extensively used in many fields, viz., prediction and controlling of flyrock in blasting operation (Monjezi et al. 2011). predicting flyrock distance caused by blasting operation (Ghasemi et al. 2014), predictive models for pot-hole depth in underground coal mining (Lokhande et al. 2014), to predict settlement under embankment load using soft soil properties together with various geometric parameters as input for each stone column (SC) arrangement and embankment condition (Chik et al. 2014), and to predict the elastic properties (Poisson's ratio and Young's modulus) of the schistose rocks from unconfined strength (UCS and tensile strength) (Khandelwal and Singh 2011). ANN has also found its wider application in the field of ground vibration due to blasting and waste dump stability (Singh and Singh 2005; Khandelwal and Singh 2006; Khandelwal and Singh 2002). Further, this artificial intelligence technique has been successfully used in modeling and predicting ventilation methane emissions of longwall mines (Karacan 2008).

In addition, attempts have also been made to classify the coals according to their proneness to spontaneous heating by multilayer perceptron (MLP) classifier to validate the findings.

The multilayer perceptron has been applied in the field of air quality prediction, classification of satellite images to distinguish between clouds and ice or snow, and classification of atmospheric circulation patterns (Gardner and Dorling 1998). Further examples of its applications include prediction of surface ozone concentrations in an industrialized area (Yi and Prybutok 1996), prediction of the existence of tornadoes (Marzban and Stumpf 1996), and vision problems: recognition and pose estimation of 3D objects from a single 2D perspective view, and handwritten digit recognition (Khotanzad and Chung 1998).

Experimental investigation

Seventy-eight (78) coal samples covering fiery and non-fiery seams of 13 mining companies of India were collected for this investigation (Ray 2013). The companies are Eastern Coalfields Ltd. (ECL), Bharat Coking Coal Ltd. (BCCL), Central Coalfields Ltd. (CCL), Mahanadi Coalfields Ltd. (MCL), South Eastern Coalfields Ltd. (SECL), Northern Coalfields Ltd. (NCL), Western Coalfields Ltd. (WCL), North Eastern Coalfields (NEC), Singareni Collieries Company Ltd. (SCCL), IISCO Steel Plant (ISP) SAIL, Monnet Ispat & Energy Ltd., Neyveli Lignite Corporation (NLC), and Tata Steel Ltd. Location of collected coal samples extends over Raniganj, Jharia, Karanpura, Ramgarh, Bokaro, Ib Valley, Raigarh, Chirimiri, Son Valley, Wardha Valley, Kamptee, Singrauli, Pranhita-Godavari Valley, Bikaner, Neyveli, and Makum coal basins. Details of coal samples, i.e., sample code, name of the mine and the seam, and mining company are presented in Table 1.

The coal samples were collected from 55 mines by following Channel Sampling procedure (Peters 1978; IS 436 1964) and brought to the laboratory in sealed condition for analysis. Samples were ground and sieved to suitable size (−212 μm) making necessary coning and quartering. Samples were prepared for various analyses, namely, proximate (moisture, volatile matter, ash, and fixed carbon), ultimate (carbon, hydrogen, nitrogen, sulphur, and oxygen), and petrographic analyses (vitrinite, inertinite, liptinite, and mineral matter content). The proximate, ultimate, and petrographic analyses were carried out by following standard procedures (IS 1350- Part 1 1969; ASTM D 5373–93 1993; ICCP 1971; ICCP 1994; IS 9127 Part I 1979; IS 9127 Part II 1979). Crossing point temperature (CPT) of 78 coal samples was determined by standard procedure as practiced in India (Panigrahi et al. 2000). An electrochemical method called wet oxidation potential is also described in detail to find out susceptibility index of coal for the purpose of its identification and classification.

Wet oxidation potential analysis

Wet oxidation potential analysis was carried out with potassium permanganate ($KMnO_4$) as oxidizer in potassium hydroxide (KOH) solution. One hundred milliliters of such chemical mixture was taken in a beaker, and a calomel reference electrode and a carbon electrode were immersed in it. After attaining a stable reading, the potential difference, i.e., electromotive force (EMF), in millovolts, was measured between these electrodes by using a digital millivoltmeter. Equivalence factor of $KMnO_4$ in this case was maintained as 158.04/3=52.68. Experiments were carried out at different concentrations of $KMnO_4$, viz., 0.05, 0.1, 0.15, and 0.2 N in 1 N KOH and at 27, 40, and 45 °C. With a combination of different concentrations of $KMnO_4$ and temperature, 12 experiments were carried out for each coal sample. In total, 936 experiments were carried out using 78 coal samples. A 0.5-g coal sample of −212-μm size was added in the chemical mixture and was continuously stirred using a magnetic stirrer. The potential difference was recorded over a period of time until a nearly constant value was attained. Temperature of the mixture was measured with a calibrated temperature recorder. Potential difference and temperature were recorded at an interval of 1 min. Each experiment takes about an hour. The experimental setup for wet oxidation potential method is shown in Fig. 1. The difference between potential difference (PD) of the mixture before adding coal sample and after its complete oxidation was calculated for each sample. Total time taken for each experiment was recorded and thus rate of reduction of potential difference was calculated. This rate of reduction of potential difference (RPD) was considered as a parameter for susceptibility of coal to spontaneous combustion and expressed in millivolts per minute (Ray 2013).

Results and discussion

Table 2 represents independent variables, viz., moisture (M), ash (A), fixed carbon (FC) (wt%); volatile matter (VM_{daf}), carbon (C_{daf}), hydrogen (H_{daf}), nitrogen (N_{daf}), sulphur (S_{daf}), and oxygen (O_{daf}) on dry ash free basis (daf) (wt%); and maceral content, viz., vitrinite (V_{mmf}), inertinite (I_{mmf}), and liptinite (L_{mmf}) on mineral matter free basis (vol%), and dependent variables like crossing point temperature (CPT). Table 3 details out dependent variables like rate of reduction of potential difference (RPD) in different experimental conditions. Acronym used for indicating the rate of reduction of potential difference (RPD) of different experimental conditions is as follows: RPD1, RPD2, and RPD3: RPD at 0.05 N $KMnO_4$ with 1 N KOH solution at 27, 40, and 45, respectively; RPD4, RPD5, and RPD6: RPD at 0.1 N $KMnO_4$ with 1 N KOH solution at 27, 40, and 45 °C, respectively; RPD7, RPD8, and RPD9: RPD at 0.15 N $KMnO_4$ with 1 N KOH

Table 1 Details of coal samples chosen for experiments

S No.	Mine/company	Seam	S No.	Mine/company	Seam
1	Central Kajora, ECL	RVIII	40	Churcha East, SECL	V
2	Parascole East, ECL	RVII	41	Haldibari, SECL	XB
3	Shamsunderpur, ECL	RVII	42	Kamptee OCP, WCL	VB
4	Lakhimata, ECL	Metadih	43	Saoner Mine 1, WCL	IV (M)
5	Lakhimata, ECL	BII	44	Saoner Mine 3, WCL	V
6	Jhanjra, ECL	RVIIA	45	Umrer OCP, WCL	IV
7	MIC unit Jhanjra, ECL	RVI	46	New Majri III, WCL	Majri
8	Jhanjra, ECL	RVII	47	Ghuggus OCP, WCL	Meyo Bottom
9	Kottadih Project, ECL	RV	48	Ghuggus OCP, WCL	Meyo Middle
10	Kottadih, ECL	RIII/II	49	Naigaon OCP, WCL	Meyo Bottom
11	Khaskajora, ECL	RVIIIA	50	Naigaon OCP, WCL	Meyo Middle
12	Khaskajora, ECL	RVIIIB	51	Jhingurda, WCL	Jhingurdah
13	Kumardhubi, ECL	Singpur Top	52	Jayant OCP, WCL	Turra
14	Bansdeopur, BCCL	VIII	53	Jayant OCP, WCL	Purewa Bottom
15	Victoria West, BCCL	Ramnagar	54	Jayant OCP, WCL	Purewa Top
16	Sudamdih shaft, BCCL	XI/XII	55	Amlohri OCP, WCL	Purewa Merge
17	Bastacolla, BCCL	0	56	Amlohri OCP, WCL	Turra
18	Bastacolla, BCCL	I	57	Tipong, NEC	20 Feet
19	Bastacolla, BCCL	II	58	Tipong, NEC	60 Feet (Bottom)
20	Moonidih, BCCL	XVI (T)	59	Tipong, NEC	60 Feet (Top)
21	Mudidih, BCCL	IX	60	Tirap OCP, NEC	8 Feet
22	Kalyani, CCL	Karo (Major)	61	Tirap OCP, NEC	60 Feet (Top)
23	Argada, CCL	I	62	Tirap OCP, NEC	20 Feet
24	Argada, CCL	J	63	Kakatiya LW, SCCL	I
25	Hesagora, CCL	X Bottom	64	Kakatiya LW, SCCL	IA
26	Churi, CCL	Lower Bachra	65	Kakatiya LW, SCCL	II
27	KD Hessalong, CCL	Dakra	66	Kakatiya LW, SCCL	III
28	Kuju, CCL	VII	67	Adriyala Shaft, SCCL	I
29	Lilari OCP, MCL	Lajkura Top	68	RK New Tech incline, SCCL	1A
30	Belpahar OCM, MCL	IB	69	Sijua, Tata Steel Ltd.	XIII
31	Belpahar OCM, MCL	Rampur Top	70	Sijua, Tata Steel Ltd.	XIV
32	Belpahar OCM, MCL	Rampur Bottom	71	6&7 Pits, Tata Steel Ltd.	IX
33	Lakhanpur OCP, MCL	Lajkura Top	72	6&7 Pits, Tata Steel Ltd.	XI
34	Jagannath OCP, MCL	III	73	Milupara, Monnet Ispat & Energy Ltd.	II
35	Anjan Hill, SECL	III	74	Kondkel, Monnet Ispat & Energy Ltd.	III
36	NCPH, SECL	III	75	Chasnalla, ISP, SAIL	XII
37	Rajnagar RO, SECL	$8A_2$	76	Western Quarry, ISP, SAIL	XIII/XIV
38	5&6 Incline, SECL	Index	77	Neyveli Mine 1A, NLC	Lignite
39	Churcha West, SECL	V	78	Barsingsar lignite, NLC	Lignite

S - Sample

solution at 27, 40, and 45 °C, respectively; RPD10, RPD11, and RPD12: RPD at 0.2 N $KMnO_4$ with 1 N KOH solution at 27, 40, and 45 °C, respectively.

Values of independent variables and CPT of 78 coal samples are shown in statistical form in Table 2. Minimum, maximum, mean, and standard deviations of all variables are furnished in

Table 2. Repeatability of experimental results was verified with three coal samples, carrying out five experiments each for a sample. Sample No. 13 (Kumardhubi Colliery, Singhpur top seam, ECL) with 0.2 N $KMnO_4$ in 1 N KOH solution at 40 °C gives PD of 62, 61.1, 60.5, 61.7, and 60.9 mV whereas Sample No. 16 (Sudamdih Shaft Mine, XI/XII seam, BCCL) with 0.1 N $KMnO_4$ in 1 N KOH solution at 27 °C shows PD of 48.1, 47.6, 47.1, 47.4, and 47.0 mV. Further, with 0.2 N $KMnO_4$ in 1 N KOH solution at 40 °C, Sample No. 46 (New Majri III, Majri Seam) gives PD of 121.3, 119.7, 120.5, 118.5, and 119.1 mV. So, standard deviation of these three samples comes out to be 0.54, 0.39, and 0.99, respectively. The coefficients of variation of aforementioned samples are calculated as 0.0088, 0.0082, and 0.0083, respectively.

In order to determine the best combinations of experimental conditions to achieve optimum results in wet oxidation potential method, results are first analyzed by principal component analysis and then by artificial neural network analysis.

Principal components analysis

Principal components analysis (PCA) was carried out for finding out the influencing parameters in susceptibility of coal to spontaneous heating. Statistica 7.1 software was used for PCA. The PCA was performed with the data obtained from proximate, ultimate, and petrographic analyses and RPD (Smith 2002). This analysis reduces the dimensionality of a data set while retaining as much of the variance in the data set as possible (Karacan and Goodman 2008; Ray et al. 2014). Most of the variance in data set is retained in the first components that contribute to variance to a greater degree. In PCA, the variables considered were moisture on analytical basis; volatile matter yield on dry ash free (daf) basis; ash, fixed carbon, carbon, hydrogen, and oxygen on daf bases, respectively; and vitrinite, inertinite, and liptinite content on mineral matter free bases, respectively. The total sulphur content of maximum number of samples is less than 1.90 wt% (except three coal samples where the values are 7.18, 5.04, and 5.07 wt%). Further, nitrogen has no effect on the spontaneous heating tendency of coal. Therefore, these parameters are not taken into consideration in this analysis. Along with other variables, susceptibility indices RPD1, RPD2, RPD3, RPD4, RPD5, RPD6, RPD7, RPD8, RPD9, RPD10, RPD11, and RPD12 were considered one at a time in PCA. In short, this analysis was performed considering ten variables from intrinsic parameters and one variable from susceptibility index. Thereby, this analysis was performed 12 times. For convenience of presentation, only one result (RPD12 as susceptibility index) is shown.

Table 4 depicts the results of the principal components analysis performed on 11 variables. It can be seen that all variance in the data are represented by 11 principal components (PCs). However, approximately 85 % of the total variance in the data can be represented by the first four PCs. The individual contributions of the remaining seven PCs are small, and their total contribution is only 15 % of the total variance. Table 4 also lists out the eigenvalues, which show the proportion by which an eigenvector's magnitude is changed. The eigenvectors with the largest eigenvalues represent the dimensions with the strongest correlation in the data set. This data set shows that the highest correlations are also in the first four PCs. Thus, the first four PCs were selected for the principal component matrix. Table 5 shows the loadings, which indicates the influence of the variables in these four PCs. Loadings close to 1 indicate stronger correlations. Figure 2 shows the correlation circle for the factor loadings of the first two

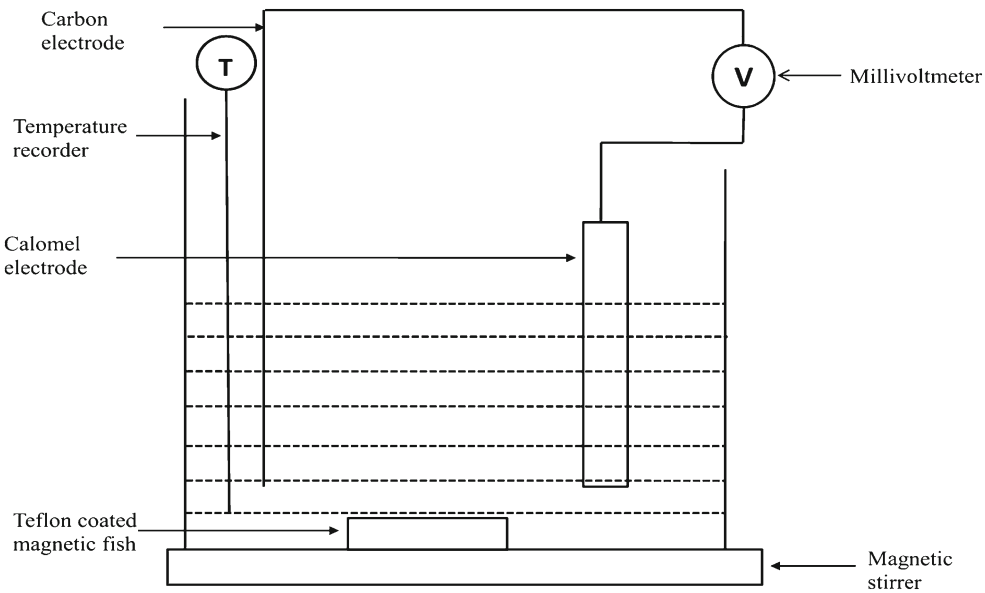

Fig. 1 Experimental setup for wet oxidation potential method (after Ray 2013)

Table 2 Variables and their units obtained from different experimental investigation

Variable	Unit	Minimum	Maximum	Mean	Std. dev.
Independent					
Moisture	%	0.4	15.71	5.20	4.08
Ash	%	0.71	38.46	16.18	8.84
Volatile matter	%	18.62	55.22	38.44	8.13
Fixed carbon	%	27.94	70.28	48.52	9.17
Carbon	%	70.02	89.56	80.62	4.58
Hydrogen	%	4.73	8.25	6.10	0.84
Nitrogen	%	0.95	2.54	1.76	0.33
Sulphur	%	0.3	7.18	1.02	1.06
Oxygen	%	1.16	19.12	10.44	4.01
Vitrinite	%	21.51	84.79	64.32	11.69
Inertinite	%	8.69	78.49	31.33	12.34
Liptinite	%	0	33.76	4.24	4.60
Dependent					
Crossing point temperature	°C	125	179	141.74	12.03

Volatile matter, carbon, hydrogen, and oxygen are on dry ash free bases and vitrinite, inertinite, and liptinite are on mineral matter free bases

components. It also shows that independent variables like moisture on analytical basis, volatile matter yield on daf basis, and hydrogen and oxygen on daf bases, and dependent variables like RPD12 are far from the center and are close to each other. Therefore, these variables are grouped together based on their weights and are significantly correlated. Further, RPD12 and fixed carbon on daf basis are on opposite sides of the center, so they are negatively correlated. However, variables like carbon, inertinite on mineral matter free basis, ash yield, and vitrinite on mineral matter free basis are orthogonal to variable RPD12. So there is no correlation between them. Liptinite on mineral matter free basis is close to the center, suggesting that its information can be better represented by other axes.

Levenberg–Marquardt model for standardizing RPD index

After identifying the variables having correlation with them by principal components analysis, results are analyzed by Levenberg–Marquardt (LM) algorithm of artificial neural network (Yu and Wilamowski 2010) in order to determine the best combinations of experimental conditions to achieve optimal results in wet oxidation potential method. The Levenberg–Marquardt (LM) algorithm is the most widely used optimization algorithm. This was independently developed by Kenneth Levenberg and Donald Marquardt. It provides a numerical solution to the problem of minimizing a non-linear function. It is found to be the fastest method for training moderate-size feed-forward neural networks. It has stable convergence. It also has an efficient implementation in MATLAB software, since the solution of the matrix equation is a built-in function. So its attributes become even more pronounced in a MATLAB environment. The network is a two-layer feed-forward network. A two-layer feed-forward network with sigmoid hidden neurons and linear output neurons can fit multidimensional mapping problems arbitrarily well, while consistent data and enough neurons are provided in its hidden layers. LM optimization algorithm has less iteration than traditional back-propagation (BP) and other improved algorithm, while its convergence rate is faster and precision is higher than that of others. Therefore, the LM optimization algorithm has certain superiority in the learning of BP network. Among simulation tool functions in the neural network of MATLAB, LM is taken as default training function in the BP neural network.

The LM algorithm is an iterative technique that locates a local minimum of a multivariate function that is expressed as the sum of squares of several non-linear, real-valued functions. It has become a standard technique for non-linear least squares problems, widely adopted in various disciplines for dealing data fitting applications.

The total (net) input to a neuron and its output are calculated using a transfer function, or axon. This is sometimes called a "squashing function" (Eberhart and Dobbins 1990). since it compresses the output range between either 0 and 1 or −1 and 1, depending on the choice of the transfer function. While there are various transfer functions, the hyperbolic tangent axon (Tenhaxon) and sigmoid functions are generally used as the non-linear axons. In the present study, sigmoid function is used.

The process of finding a suitable set of weights is called "training." Training is one of the most important steps in the development of the neural network. Based on the training method, neural networks are classified as either supervised

Table 3 Experimental results of wet oxidation potential analysis in millivolts per minute

S No.	RPD1	RPD2	RPD3	RPD4	RPD5	RPD6	RPD7	RPD8	RPD9	RPD10	RPD11	RPD12
1	4.97	5.98	6.40	4.81	8.00	7.99	5.31	8.67	9.07	5.99	5.85	7.64
2	5.22	5.64	6.21	6.01	7.20	7.95	5.38	7.54	9.58	5.77	8.29	8.17
3	4.95	6.05	4.91	5.18	7.54	8.51	5.21	5.72	6.31	5.78	6.33	8.37
4	1.02	1.19	1.26	1.94	2.56	3.96	1.58	1.81	2.52	1.48	1.63	1.81
5	1.71	2.00	1.16	1.84	2.04	1.94	1.19	2.16	2.17	1.96	1.20	1.58
6	1.38	2.70	3.72	2.56	4.62	7.61	3.80	6.71	5.19	5.15	10.70	13.79
7	1.80	3.51	3.12	2.86	3.93	4.39	5.71	5.14	3.99	8.28	12.31	11.33
8	2.52	9.75	13.05	2.83	5.27	4.45	3.41	5.50	5.96	11.58	12.45	12.08
9	3.64	1.91	1.75	4.72	4.87	6.22	4.98	4.85	6.33	6.68	8.92	7.79
10	1.97	7.21	9.85	3.17	2.79	3.16	2.98	3.41	3.55	3.57	4.90	5.54
11	8.87	9.30	8.83	2.39	2.81	3.51	3.96	2.58	14.65	5.03	6.05	8.12
12	6.57	7.78	10.35	9.88	11.45	10.04	10.74	10.88	6.44	4.72	15.26	6.69
13	1.40	1.46	1.46	2.23	1.51	1.20	1.32	2.48	3.07	1.76	2.00	2.50
14	1.35	1.23	1.24	1.14	1.20	1.52	0.83	1.87	1.57	1.44	0.93	1.78
15	1.91	1.99	1.83	1.80	2.16	3.17	2.37	2.12	2.67	1.92	2.18	2.47
16	1.00	1.43	1.14	0.76	1.10	0.92	1.27	1.11	0.92	1.04	1.45	1.32
17	1.16	2.59	2.84	0.97	1.80	1.92	1.22	1.93	1.95	1.34	1.91	1.93
18	1.53	2.05	1.47	1.52	2.78	2.79	1.16	1.73	1.53	1.22	1.82	2.18
19	1.12	1.53	2.04	0.83	0.79	1.30	1.22	1.97	1.35	1.68	1.70	1.73
20	1.00	1.35	1.44	0.86	1.42	1.54	1.10	2.28	1.91	1.13	1.79	2.35
21	0.84	1.39	2.46	1.35	1.68	1.80	1.48	1.47	1.82	1.55	2.39	2.02
22	0.98	1.25	1.35	1.20	2.32	2.60	1.03	2.68	2.26	0.89	1.44	1.30
23	2.77	3.16	4.55	3.97	5.81	6.23	3.26	4.42	4.86	2.25	4.10	3.70
24	2.73	4.40	4.25	3.18	5.61	5.21	3.17	5.24	5.80	3.22	5.28	5.18
25	1.97	3.20	3.20	2.72	3.92	4.00	1.99	3.68	3.65	2.08	2.67	3.45
26	3.44	4.79	4.61	4.32	5.98	6.53	5.09	7.01	7.28	6.38	9.72	10.18
27	3.00	4.92	4.93	4.14	7.16	6.44	4.93	6.63	8.28	5.24	9.33	8.51
28	2.17	3.49	3.31	2.01	2.72	3.15	1.81	3.06	2.68	2.01	2.59	2.61
29	6.13	9.89	9.88	7.39	9.07	10.65	6.77	10.61	11.22	6.12	15.02	14.26
30	4.55	5.17	5.89	5.84	8.38	8.59	5.82	8.89	8.51	6.54	6.56	5.81
31	3.71	6.47	5.56	5.59	8.75	8.85	5.93	8.19	8.55	6.93	6.61	8.01
32	3.92	5.09	4.80	5.34	6.86	7.39	6.59	8.54	7.96	6.33	7.60	8.69
33	4.60	4.89	5.29	5.42	11.38	10.92	7.25	10.43	11.72	6.23	8.00	9.75
34	8.13	6.77	5.88	6.51	6.09	6.29	5.15	5.48	5.38	5.21	7.10	8.72
35	3.82	4.35	3.98	2.89	3.70	4.75	4.96	6.23	6.55	3.82	6.45	6.49
36	2.45	3.11	3.37	3.35	5.07	6.29	5.06	6.82	9.71	5.26	7.92	6.85
37	4.30	4.74	5.19	3.55	4.91	5.01	3.60	5.90	6.14	2.83	5.45	5.93
38	3.55	6.56	6.97	3.59	6.46	6.49	5.50	7.44	9.39	5.41	6.00	6.46
39	1.80	3.34	2.70	1.48	2.67	2.37	2.09	2.62	2.16	1.96	2.69	2.72
40	1.81	2.59	2.35	1.70	2.29	2.53	1.58	1.92	1.77	1.96	2.21	2.08
41	2.29	3.99	3.80	3.85	6.41	5.82	2.91	5.65	5.74	3.96	6.73	6.05
42	3.92	5.37	7.28	5.80	7.23	11.99	8.23	9.03	8.65	9.30	8.42	10.77
43	7.63	10.21	5.02	9.09	8.69	7.46	10.82	11.73	13.02	10.94	9.86	10.71
44	3.16	5.03	6.21	5.40	7.52	11.67	3.93	9.37	9.16	7.66	10.61	15.30
45	3.56	4.23	4.38	3.68	5.63	5.78	4.44	6.76	6.84	4.85	8.58	19.03
46	8.42	8.23	10.06	10.73	12.30	12.88	9.09	11.77	10.55	4.81	10.91	11.48
47	5.54	12.56	10.70	10.28	11.43	12.02	9.20	11.71	11.92	7.60	9.70	12.18
48	9.08	11.94	11.70	10.12	14.77	14.49	6.42	11.77	12.43	6.11	9.88	10.84
49	7.21	8.56	10.11	8.70	9.93	10.55	7.56	11.32	11.75	8.11	10.74	11.85
50	4.19	7.18	5.05	6.60	10.83	12.94	6.71	9.42	9.22	8.23	9.43	8.36
51	7.06	11.34	13.13	4.45	6.44	6.69	8.34	8.78	8.43	5.22	9.55	10.86

Table 3 (continued)

S No.	RPD1	RPD2	RPD3	RPD4	RPD5	RPD6	RPD7	RPD8	RPD9	RPD10	RPD11	RPD12
52	7.25	6.56	5.48	6.17	8.04	8.43	4.47	16.31	13.98	8.14	12.26	11.98
53	4.62	4.55	6.79	4.10	6.89	4.40	3.86	5.56	4.09	6.24	7.33	11.23
54	3.80	4.43	6.05	4.20	5.81	5.16	4.25	4.97	5.72	5.39	6.15	9.02
55	4.97	7.05	7.69	5.43	7.42	7.35	5.01	5.89	13.99	12.06	15.66	9.45
56	4.25	5.21	6.13	4.26	5.63	4.15	4.51	5.86	5.93	6.16	7.44	7.89
57	3.24	3.69	4.80	1.86	2.59	3.18	2.00	2.82	2.42	1.91	2.68	2.60
58	1.65	1.93	2.29	1.15	1.85	1.89	1.33	1.65	1.50	1.43	1.78	2.17
59	1.66	2.51	3.00	1.50	2.05	2.41	1.43	2.07	2.94	1.43	2.85	3.06
60	2.78	4.27	4.21	2.40	4.57	4.28	2.21	2.75	2.82	2.15	3.23	3.23
61	1.85	2.76	2.81	1.51	2.14	2.64	1.55	2.36	2.19	1.77	1.92	3.42
62	1.92	1.92	1.77	1.42	1.71	1.89	1.41	1.93	1.97	1.42	1.72	1.87
63	4.32	5.60	6.75	2.78	4.59	6.72	4.23	7.28	8.36	4.62	8.24	8.43
64	3.66	6.80	4.21	4.46	5.92	6.55	5.05	6.97	6.73	3.79	7.52	8.13
65	2.92	4.62	4.54	3.64	5.87	6.18	3.28	6.74	6.18	3.24	5.40	6.22
66	2.67	3.18	2.76	3.19	4.61	6.19	4.19	6.19	6.75	3.40	4.24	7.12
67	3.79	5.12	4.10	4.55	4.60	6.69	3.52	6.77	6.25	3.32	7.22	8.21
68	2.73	4.34	5.57	5.24	6.76	7.40	4.34	6.96	7.67	6.13	9.85	10.41
69	1.04	1.46	1.68	0.83	2.07	1.55	0.94	1.39	1.89	1.17	2.10	1.75
70	1.36	1.77	1.41	1.10	2.17	2.32	1.22	1.75	1.89	1.21	1.94	2.19
71	1.18	2.01	1.70	0.87	1.87	1.98	1.22	1.75	1.81	1.16	1.69	2.78
72	1.33	1.77	1.66	1.29	1.79	1.91	1.86	1.99	2.44	1.47	1.95	2.09
73	4.25	5.93	7.86	4.79	8.78	9.65	5.72	6.60	7.80	5.82	11.08	14.39
74	2.13	4.00	3.61	1.93	4.70	3.99	6.82	8.64	7.66	5.48	8.47	7.23
75	1.37	1.31	1.20	2.39	2.13	2.95	1.43	1.18	1.25	1.82	1.98	2.47
76	1.28	2.03	1.27	1.54	2.13	2.69	1.61	1.94	2.54	0.99	2.04	1.76
77	2.97	3.85	3.12	2.98	3.11	3.17	4.62	7.56	9.17	5.51	10.05	11.30
78	3.44	6.32	7.87	3.28	3.15	3.53	7.41	7.48	8.55	5.43	8.71	12.20

or unsupervised networks (Mohaghegh 1990). The supervised training algorithm requires repeated showings (Epoch) of both input vectors and the expected outputs of the training set of the network. This is to let it learn the relations on a feedback basis. The neural network computes its output at each epoch and compares it with the expected output (target) of each input vector in order to calculate the error. Minimizing the mean square error (MSE) is the goal of the training process. The most widely used technique is propagating the error back and adjusting the initially assigned random weights to each

Table 4 Eigen values of correlation matrix, and the variances explained by PCA

PC	Eigenvalue	% Total variance	Cumulative eigenvalue	Cumulative %
1	5.44	49.42	5.44	49.42
2	1.75	15.92	7.19	65.34
3	1.27	11.57	8.46	76.90
4	0.88	8.02	9.34	84.93
5	0.68	6.21	10.02	91.13
6	0.46	4.22	10.49	95.35
7	0.31	2.81	10.80	98.16
8	0.17	1.57	10.97	99.73
9	0.03	0.23	11.00	99.96
10	0.00	0.03	11.00	99.99
11	0.00	0.01	11.00	100.00

The first four PCs represent ~85 % of the total variance

Table 5 Factor loadings of the variables in the principal component matrix for the four principal components

Variables	PC1	PC2	PC3	PC4
Moisture	0.699	−0.299	0.354	0.316
VM_{daf}	0.938	0.006	0.032	−0.052
Ash	−0.055	−0.755	−0.496	−0.110
FC	−0.815	0.494	0.181	0.011
C_{daf}	−0.897	0.018	0.115	0.300
H_{daf}	0.778	−0.078	0.147	−0.094
O_{daf}	0.858	−0.098	−0.105	−0.279
V_{mmf}	0.681	0.606	0.009	−0.075
I_{mmf}	−0.659	−0.634	0.294	−0.101
L_{mmf}	0.074	0.152	−0.808	0.447
RPD12	0.594	−0.196	0.286	0.612

Moisture (wt%; on analytical basis); VM_{daf}, volatile matter yield (wt%) on daf basis; ash yield (wt%); FC, fixed carbon (wt%); C_{daf}, H_{daf}, and O_{daf}, carbon, hydrogen, and oxygen (wt%) on daf bases, respectively; V_{mmf}, I_{mmf}, and L_{mmf}, vitrinite, inertinite, and liptinite content (vol%) on mineral matter free bases, respectively; RPD12, susceptibility index

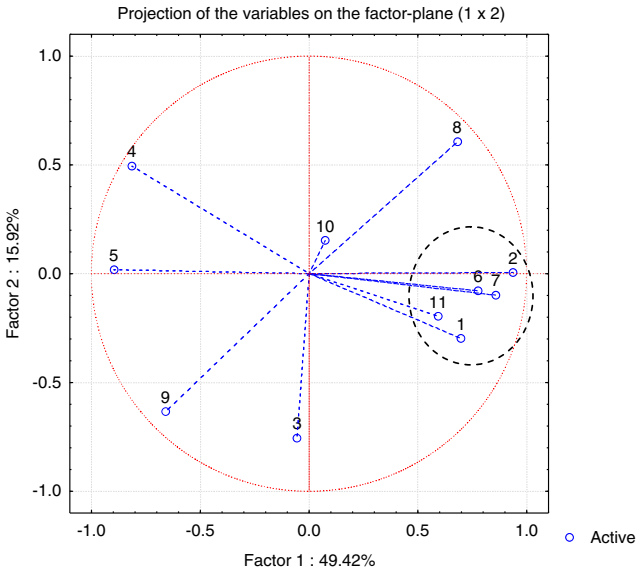

Fig. 2 Projection of variables on the factor plane

neuron. This process is called back propagation. This very technique is used in this paper.

As revealed from principal components analysis, independent variables like moisture, volatile matter yield (daf basis), and hydrogen and oxygen on daf bases and fixed carbon are considered as input parameters (five numbers) for ANN analysis. The rate of potential difference at different experimental conditions, viz., RPD1, RPD2, RPD3, RPD4, RPD5, RPD6, RPD7, RPD8, RPD9, RPD10, RPD11, and RPD12, is considered as output parameter one at a time. For each output parameter, this exercise is conducted and maximum correlation coefficient (R) and mean square error (MSE) are recorded.

Results of analysis with artificial neural network

The neural network model was trained with Levenberg–Marquardt (LM) back propagation (BP) algorithm till maximum correlation coefficient was achieved. Out of 78 data sets, 54 were considered for training (70 % of total data), 12 (15 % of total data) were considered for validation, and the remaining 12 (15 % of total data) were used for testing. Neural network fitting tool was used for data analysis purpose. The number of neurons in the fitting network's hidden layer is set as 12, after ensuring that the network is performing well after training. For each output parameter, this exercise was conducted and maximum correlation coefficient (R) and mean square error (MSE) were recorded. Note that mean square error is the average square difference between outputs and targets. Lower values are preferable as well as better, and zero means no error. Similarly, regression R value measures the correlation between outputs and targets. An *R* value of 1 indicates a close relationship whereas a 0 indicates random relationship.

Table 6 depicts the results of analysis from artificial neural network. It is revealed from Table 6 that RPD12 gives maximum correlation coefficient of 0.95 and mean square error of 1.83. For ease of presentation, regression plot for susceptibility index RPD12 is shown in Figure 3. Therefore, it is recommended that rate of reduction of potential difference (RPD12) in WOP method, using 0.2 N $KmnO_4$ solution with 1 N KOH at 45 °C, should be used for determining the susceptibility of coal to spontaneous combustion. It is also concluded that for classification of coals according to their proneness to spontaneous heating, susceptibility index RPD12 is considered as one of the parameters. Coals are classified according to their proneness to spontaneous heating and are described in subsequent paragraphs (section Classification of coals using classifier).

Comparison between RPD12 and CPT

Ensuring RPD12—a suitable susceptibility index in WOP method by ANN—the next question comes to a practicing

Table 6 Results of analysis with artificial neural network

Indices	RPD1	RPD2	RPD3	RPD4	RPD5	RPD6	RPD7	RPD8	RPD9	RPD10	RPD11	RPD12
R	0.87	0.87	0.85	0.86	0.85	0.83	0.86	0.89	0.91	0.91	0.90	0.95
MSE	1.00	1.77	2.50	1.76	2.69	3.44	1.83	2.47	2.25	1.46	2.77	1.83

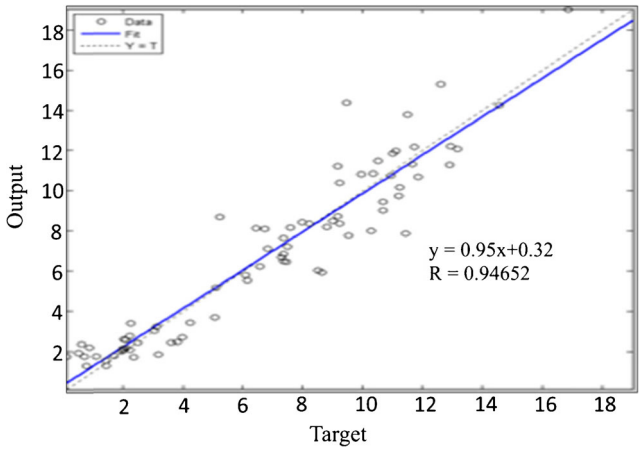

Fig. 3 Regression plot for RPD12

mining engineer whether this susceptibility index is better than CPT—a thermal method widely used in India to determine susceptibility of coal to spontaneous heating.

Table 7 represents correlation coefficients obtained from correlation analysis between CPT and intrinsic parameters like moisture (M), volatile matter on daf basis (VM_{daf}), fixed carbon, hydrogen (H_{daf}), and oxygen (O_{daf}) on daf bases, and a combination of moisture and volatile matter, and oxygen and hydrogen. This correlation analysis was performed with Design Expert 7.0.0 software. Similar analysis was carried out with RPD12. Results are depicted in Table 7. It reveals from Table 7 that poor correlation coefficients are observed when susceptibility index (RPD12) is correlated with petrographic constituents. Therefore, these are not considered for comparison purpose.

The following points are noteworthy while comparing RPD12 and CPT (Table 7):

- Overall improvement of correlation coefficients is noticed while analysis is done with RPD12.
- Maximum improvement in correlation coefficient is observed while correlating with moisture. In case of RPD12, it is 0.94, while in case of CPT, it is 0.62.
- While carrying out correlation studies with FC, correlation coefficient *r* is found to be 0.75 in case of CPT analysis, and RPD12 analysis depicts its value as 0.78.
- Improvement in correlation coefficient is also observed in case of H_{daf} and O_{daf}. While correlation is done with hydrogen, CPT analysis shows that *r* is 0.62, and RPD12 analysis shows it to be 0.65. Similarly, when correlation is done with oxygen, CPT analysis shows that the *r* is 0.74, and RPD12 analysis shows it to be 0.77.
- Correlation coefficient *r* is also obtained combining M and VM_{daf} for both the analyses. CPT analysis depicts its value 0.85, and RPD12 analysis gives it as 0.94.
- Considering O_{daf} and H_{daf} as two independent variables, correlation analysis is made with CPT as well as RPD12. In case of CPT, *r* is found to be 0.75, and in case of RPD12, its value is 0.80.
- Both the analysis results indicate that RPD12 gives the highest correlation coefficient in the maximum number of cases.

Classification of coals using classifier

After comparing RPD12 with CPT and finding out RPD12 as a better susceptibility index than CPT, efforts were made to classify the coal samples according to their spontaneous heating tendency using RPD12 as one of the parameters for further validation of the findings. Multilayer perceptron (MLP) classifier was used in this recognition process. It is worth mentioning that in this process, suitable intrinsic parameters (i.e., M, VM, and FC) were also taken into consideration.

A multilayer perceptron (MLP) is a feed forward artificial neural network model that maps sets of input data onto a set of appropriate outputs. An MLP consists of multiple layers of nodes in a directed graph, with each layer fully connected to the next one. Except for the input nodes, each node is a neuron (or processing element) with a non-linear activation function. MLP utilizes a supervised learning technique called backpropagation for training the network. MLP is a modification of the standard linear perceptron and can distinguish data that are not linearly separable. MLP architecture has a single hidden layer and the network transfer function $y=f(x)$ is given by $\boldsymbol{y}=\boldsymbol{W}^{0}\varphi(\boldsymbol{W}^{H}\boldsymbol{x})$, where $\boldsymbol{x}$ is the input vector, $\boldsymbol{W}^{H}$ is the weight matrix connecting input and hidden units, and $\boldsymbol{W}^{0}$ is the weight matrix connecting hidden and output units. The activation function φ, normally a sigmoidal, introduces a non-

Table 7 Correlation coefficients obtained from CPT and RPD12 analysis

Sl. No.	Intrinsic Characteristics	Susceptibility indices	
		CPT	RPD12
1	M	0.62	0.94
2	VM_{daf}	0.78	0.74
3	FC	0.75	0.78
4	H_{daf}	0.62	0.65
5	O_{daf}	0.74	0.77
6	M and VM_{daf}	0.85	0.94
7	O_{daf} and H_{daf}	0.75	0.80

M moisture, VM_{daf} volatile matter yield on daf basis, *FC* fixed carbon, H_{daf} and O_{daf} hydrogen and oxygen on daf bases

Table 8 Confusion matrix for M, VM, FC, and RPD12 data for MLP classifier

Category	Highly	Poorly	Moderately
Highly	44	0	0
Poorly	2	16	0
Moderately	2	0	6

linear effect at the hidden units. To arrive at the optimal $\boldsymbol{W^H}$, $\boldsymbol{W^0}$ weights, MLPs are trained by minimizing the sum-of-squares error (SSE) function

$$E(W) = \sum_{n=1}^{N} \frac{\|f(x_n) - t_n\|^2}{2}$$

with t_n being the target associated to the nth input. MLPs are capable of approximating any continuous function g: $R^D \rightarrow R^M$ to any given accuracy, provided that sufficiently many hidden units are available; in particular, a trained MLP $f(x)$ can be expected to approximate the optimal minimum square estimator (Freeman and Skapura 1991).

Training and testing

As per field observations, 48 coal samples are considered belonging to fiery seams. As per Coal Mines Regulations 1957, "fiery seam" means a seam in which a fire or spontaneous heating exists in the workings below ground or in open cast workings lying within the precincts of a mine. Twenty samples are from non-fiery/poorly susceptible seams. Therefore, the rest ten samples may be assumed moderately susceptible. Sample No. 1, 2, 3, 6, 7, 8, 9, 10, 11, 12, 26, 27, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 63, 64, 65, 66, 67, 68, 73, 74, 77, and 78 are from fiery seams whereas sample No. 4, 5, 13, 14, 16, 17, 18, 19, 20, 21, 22, 39, 40, 62, 69, 70, 71, 72, 75, and 76 belong to non-fiery seams. The remaining ten samples, viz., sample No. 15, 23, 24, 25, 28, 57, 58, 59, 60, and 61, are from moderately susceptible group (Table 1). MLP classifier has been used to validate the findings. These results are tested by Weka (Waikato 2015). Weka contains a collection of visualization tools and algorithms for data analysis and predictive modeling together with graphical user interfaces.

The data contains 48 samples of highly susceptible class having four attributes, viz., M, VM, FC, and RPD12. Similarly, the other classes, i.e., poorly susceptible class, includes 20 samples and moderately susceptible one includes 10 samples with the same number of attributes. Ten percent (10 %) of the randomly chosen samples (four samples from highly susceptible, two samples from poorly susceptible, and two samples from moderately susceptible group) were considered as the training set covering all the three classes, and subsequently 90 % samples were considered as the test set (i.e., without class label supplied to the system).

The samples used for training are chosen at random to avoid any biasness. It may be mentioned here that training operation with classifier is done using labeled samples (i.e., known class). The training of the network is performed in the following manner:

Once the classifier is trained properly with known class labels, testing is done with 90 % samples, i.e., with a total 70 samples to predict class for each sample. All these operations are done with the platform of Weka classifiers. The classification performance is measured in terms of accuracy predicted by the system considering four attributes together, i.e., M, VM, FC, and RPD12.

Classification/recognition score

The recognition score is generated in the following fashion. After the training is over, the test data is applied one at a time, without supplying the class label to the system. The system then predicts its class as output. If the prediction is a hit (i.e., correctly classified), the number of samples correctly

Table 9 Classification of coals with different attributes

Attributes	Training		Testing	
	Correct classification %	Incorrect classification %	Correct classification %	Incorrect classification %
VM, M, RPD12, FC, H, O	100	0	90	10
VM, M, RPD12	100	0	87.1429	12.8571
VM, M, RPD12, FC	100	0	94.2857	5.7143
VM, M, RPD12, H	100	0	91.4286	8.5714
VM, M, RPD12, O	100	0	90	10

M moisture, *VM* volatile matter yield on daf basis, *FC* fixed carbon, *H* hydrogen, *O* oxygen, *RPD12* susceptibility index

Table 10 RPD12 value range for different category of samples

Group	Status	RPD12 value range, mV/min
1	Poorly susceptible	1.30–2.78
2	Moderately susceptible	2.17–5.18
3	Highly susceptible	5.54–19.03

classified is increased by 1; otherwise, it is a miss and the corresponding counter (i.e., the number of incorrectly classified samples) is incremented by 1. In this manner, the confusion matrix is generated for measuring the recognition/classification score. An illustration of the confusion matrix using MLP classifier is shown below in Table 8.

The first row in the confusion matrix contains 44 correctly classified samples (predicted by the system) without any misclassification of any sample for this group. The second row in the confusion matrix contains 16 correctly classified samples of poorly susceptible class (as predicted by the system) with 2 misclassified samples (i.e., misclassified as highly susceptible group sample). Similarly, in the third row of the confusion matrix, the number of correctly classified samples of moderately susceptible group is 6 and number of incorrectly classified samples is 2 (as categorized by the system as highly susceptible group). Hence, the total recognition/classification score is computed as

$$\%\ correct\ classification = \left(No.\ of\ correctly\ classified\ samples \Big/ total\ no.\ of\ test\ sample\right)*100$$

The results of the classification are presented in Table 9. From Table 9, it may be observed that the recognition score is highest, i.e., 94.29 % when four attributes, viz., VM, M, RPD12, and FC, are used for classification. The recognition score is lowest when classification is done with three attributes, viz., VM, M, and RPD12.

- It is clear that RPD12 values of the samples of highly susceptible group range between 5.54 and 19.03, whereas for poorly susceptible group, they vary from 1.30 to 2.78, and for moderately susceptible group, they vary from 2.17 to 5.18. However, a few samples of moderately susceptible group (lying within the range of 2.17–2.78) overlap with the samples of poorly susceptible group as outliers, leading to misclassification. With large population of samples, the misclassification may possibly get reduced further.

The overlapping nature of the samples can be reduced if the same model is tested for a large number of samples having different ranges of their intrinsic properties. Therefore, the classification is made as given in Table 10.

Tenfold cross-validation

Cross-validation is a model validation technique for assessing how the results of an analysis will generalize to an independent data set. Each round of cross-validation involves partitioning a sample of data into complementary subsets, performing the analysis on one subset (training set), and validating the analysis on the other subset (validation set or testing set). It mimics the use of training and test sets by repeatedly training the algorithm K times with a fraction $1/K$ of samples left out for testing purposes. In this case, K=10 is

Table 11 Results of tenfold cross-validation method (classification score)

S. No.	Random seed	% of Correctly classified instances	% of Incorrectly classified instances	Mean absolute error	Root-mean-square error
1.	1	94.8718	5.1282	0.0578	0.1801
2.	3	94.8718	5.1282	0.0568	0.1747
3.	9	94.8718	5.1282	0.0564	0.1739
4.	13	93.5897	6.4103	0.0597	0.1814
5.	15	94.8718	5.1282	0.0584	0.1780
6.	19	94.8718	5.1282	0.0571	0.1729
7.	25	94.8718	5.1282	0.0541	0.1686
8.	31	94.8718	5.1282	0.0598	0.1791
9.	37	94.8718	5.1282	0.0589	0.1798
10.	43	94.8718	5.1282	0.0597	0.1781
Std. Deviation		0.4054	0.4054	0.0018	0.0040
Average		94.7436	5.2564	0.0579	0.1767

used, i.e., tenfold cross-validation. In each experimental run, nine folds are used for training and the remaining one fold is used for testing. Therefore, training set consists of 90 % data and test set consists of 10 % data.

The tenfold cross-validation is performed on whole dataset with four features (M, VM, RPD12, and FC). To reduce variability, multiple rounds of cross-validation are performed using different random partitions, and the validation results are averaged over the rounds. Classification results reported here are based on MLP classifier. In this case, ten runs of tenfold cross-validation method with random seed for percent split (seed value is taken odd numbers like 1, 3, and 9 for ten runs) are used that produces different random folds for each run. Finally, the standard deviation (SD), mean absolute error, and root-mean-square error for all runs are calculated.

The results are depicted in Table 11. As observed from the Table 11, the standard deviation, mean absolute error, and root-mean-square error are 0.4054, 0.0018, and 0.0040, respectively, averaged over ten runs. It is to be noted that results with low variations among different runs are preferred. The tenfold cross-validation results indicate the consistent performance of the MLP classifier over the chosen features.

Conclusions

The following conclusions emerge from the present investigations:

- PCA analysis results indicate that intrinsic properties of coal, specifically moisture, volatile matter yield, hydrogen, and oxygen are positively correlated with susceptibility index, RPD, and fixed carbon is negatively correlated with RPD. Further, ash yield, carbon, and vitrinite, inertinite and liptinite on mineral matter free basis have no correlation with RPD.
- A comparison between correlation coefficients obtained from CPT and RPD12 analysis indicates that RPD12 gives the highest correlation in maximum number of cases. So, RPD12 is a better susceptibility index than CPT.
- Artificial neural network analysis indicates that RPD12 is the best susceptibility index to get optimal results. In other words, with wet oxidation potential method, the experimental conditions should be 0.2 N $KMnO_4$ solution with 1 N KOH at 45 °C to achieve optimal results for finding out the susceptibility of coal to spontaneous combustion.
- Coal seams were classified according to their proneness to spontaneous heating with the help of different attributes using multilayer perceptron classifier with a correct classification of 94.29 %. The results are further validated by tenfold cross-validation method to show the consistent performance of the MLP classifier over the chosen features.
- As per the categorization of susceptibility of coal seams, the highly susceptible group has RPD12 values range between 5.54 and 19.03 mV/min. For the poorly susceptible group, RPD values range between 1.30 and 2.78 mV/min, and for moderately susceptible group, these range between 2.17 and 5.18 mV/min. Therefore, there exist overlapping values of RPD12 in case of poorly and moderately susceptible groups. To get precise range of RPD12 values, a large population of samples belonging to poorly and moderately susceptible group may be required.

References

ASTM D 5373–93 (1993) Standard test methods for instrumental determination of carbon, hydrogen and nitrogen in laboratory samples of coal and coke

Banerjee SC (2000) Coal categorization vis-à-vis spontaneous fire risk. In: Prevention and Combating Mine Fires, Special Indianth edn. Oxford & IBH Publishing Co. Pvt. Ltd, New Delhi, pp 67–113

Banerjee SC, Nandy DK, Banerjee DD, Sen SK (1988) Spontaneous fire risk rating of a colliery proposed to be developed by short wall method of mining. In: Proceedings of Fourth International Mine Ventilation Congress, Brisbane, Queensland, July, pp 365–373

Baris K, Kizgut S, Didari V (2012) Low temperature oxidation of some Turkish coals. Fuel 93:423–432

Beamish BB, Arisoy A (2008) Effect of intrinsic coal properties on self-heating rates. In: 12th US/North American Mine Ventilation Symposium, Wallace (ed), ISMN 978-0-615-20009-5, 149–15: pp 125–130

Beamish BB, Arisoy A (2008b) Effect of mineral matter on coal self-heating rate. Fuel 87:125–130

Behera P, Mohanty G (2009) Peroxy complex and crossing point temperature of Talcher coals—an adducer to assess the spontaneous heating combustibility character. J Sci Res 1:55–60

Carras JN, Day SJ, Saghafi A, Williams DJ (2009) Greenhouse gas emissions from low-temperature oxidation and spontaneous combustion at open-cut coal mines in Australia. Int J Coal Geol 78:161–168

Chik Z, Aljanabi QA, Kasa A, Taha MR (2014) Tenfold cross validation artificial neural network modeling of the settlement behavior of a stone column under a highway embankment. Arab J Geosci 7:4877–4887

Didari V (1988) Developing a spontaneous combustion risk index for Turkish coal mines - Preliminary studies. J Mines Met Fuels 211–215

Eberhart RC, Dobbins RW (1990) Neural network PC tools: a practical guide. Academic Press Inc., San Diego, CA

Esmaeili M, Salimi A, Drebenstedt C, Abbaszadeh M, Bazzazi AA (2014) Application of PCA, SVR, and ANFIS for modeling of rock fragmentation. Arab J Geosci.

Freeman JA, Skapura DM (1991) Neural Networks Algorithms, Applications, and Programming Techniques. Addison-Wesley Publishing Company, 401 p

Gardner MW, Dorling SR (1998) Artificial neural networks (the multilayer perceptron)—a review of applications in the atmospheric sciences. Atmos Environ 32:2627–2636

Ghasemi E, Amini H, Ataei M, Khalokakaei R (2014) Application of artificial intelligence techniques for predicting the flyrock distance caused by blasting operation. Arab J Geosci. doi:10.1007/s12517-012-0703-6

Ghosh R (1986) Spontaneous combustion of certain Indian coals—some physico-chemical considerations. Fuel 65:1042–1046

ICCP (International Committee for Coal and Organic Petrology) (1971) International handbook of coal petrology, 2nd edn. C.N.R.S, Paris

ICCP (International Committee for Coal and Organic Petrology) (1994) Vitrinite Classification. C.N.R.S, Paris

IS (Indian Standard): 436 (1964) Methods of sampling of coal and coke, pp 13

IS (Indian Standard): 1350 Part - I (1969) Methods of test for coal and coke - proximate analysis, pp 5–18

IS (Indian Standard): 9127 Part - II (1979a) Methods for petrographic analysis of coal - Preparation of coal samples for petrographic analysis; pp 4–8

IS (Indian Standard): 9127 Part -I (1979) Methods for petrographic analysis of coal, pp 5–7

Karacan CÖ (2008) Modelling and prediction of ventilation methane emissions of US longwall mines using supervised artificial neural networks. Int J Coal Geol 73:371–387

Karacan CÖ, Goodman GVR (2008) Artificial neural networks to determine ventilation emissions and optimum degasification strategies for longwall mines. In: Proc. 12th U.S./North American Mine Ventilation Syposium, pp 321–329

Kaymakci E, Didari V (2002) Relations between coal properties and spontaneous combustion parameters. Turkish J Engg Env Sci 26: 59–64

Khandelwal M, Singh TN (2002) Prediction of waste dump stability by an intelligent approach. Nat Sym, New Equipment – New Technology, Management and Safety, ENTMS, Bhubeneshwar, India, pp 38–45

Khandelwal M, Singh TN (2006) Prediction of blast induced ground vibration and frequency in opencast mines. J of Sound Vibr 289: 711–725

Khandelwal M, Singh TN (2011) Predicting elastic properties of schistose rocks from unconfined strength using intelligent approach. Arab J Geosci 4:435–442

Khotanzad A, Chung C (1998) Application of multi-layer perceptron neural networks to vision problems. Neural Comput Appl 7:249–259

Labib K, Vemuri VR (2004) An application of principal component analysis to the detection and visualization of computer network attacks. www.cs.ucdavis.edu/~vemuri/papers/pcaVisualization.pdf . Accessed on 03.03.15

Lang L, Fu-bao Z (2010) A comprehensive hazard evaluation system for spontaneous combustion of coal in underground mining. Int J Coal Geol 82:27–36

Lokhande RD, Murthy VMSR, Singh KB (2014) Predictive models for pot-hole depth in underground coal mining—some Indian experiences. Arab J Geosci 7:4697–4705

Marzban C, Stumpf GJ (1996) A neural network for tornado prediction based on Doppler radar derived attributes. J Appl Meteorol 35:617–626

Mohaghegh S (1990) Virtual-intelligence applications in petroleum engineering: Part 1-Artificial neural networks. JPT 52:64–73

Monjezi M, Bahrami A, Ali YV, Ahmad RS (2011) Prediction and controlling of flyrock in blasting operation using artificial neural network. Arab J Geosci 4:421–425

Ohlemiller TJ (2002) Smouldering Combustion. In: SEPE Fire Protection Handbook, National Fire Protection Association, Quincy, 3rd edition. MA 02269; pp 2.200-2.210

Ozdeniz AH (2010) Determination of spontaneous combustion in industrial-scale coal stockpiles. Energ Source Part A 32:665–673

Panigrahi DC, Saxena VK, Udaybhanu G (2000) A study of susceptibility of Indian coals to spontaneous combustion and its correlation with their intrinsic properties. In: Proc. First International Conference on Mine Environment and Ventilation, ISM, Dhanbad, pp 347–353.

Panigrahi DC, Sahu HB, Udayabhanu G, Saxena VK (2004) Wet oxidation method for predicting the spontaneous heating susceptibility of Indian coals. CMTM, June-August, 13–21

Peters WC (1978) Exploration and Mining Geology. John Wiley and Sons Inc, New York, pp 416–425

Ray SK (2013) Development and standardization of a method for studying the susceptibility of coal to spontaneous heating. Ph.D. Thesis, Indian School of Mines, Dhanbad, India

Ray SK, Panigrahi DC, Varma AK (2014) An electro-chemical method for determining the susceptibility of Indian coals to spontaneous heating. Int J Coal Geol 128–129:68–80

Singh TN, Singh V (2005) An intelligent approach to prediction and control ground vibration in mines. Geotech Geol Eng 23:249–262

Smith LI (2002) A tutorial on Principal Components Analysis. http://www.cs.otago.ac.nz/cosc453/student_tutorials/ principal_components.pdf . Accessed on 10.02.14

Tarafdar MN, Guha D (1989) Application of wet oxidation processes for the assessment of the spontaneous heating of coal. Fuel 68:315–317

Waikato (2015) Machine Learning Group at the University of Waikato. http://www.cs.waikato.ac.nz/ml/weka/documentation.html. Accessed on 20.02.15,

Xuyao Q, Wang D, Milke JA, Zhong X (2011) Crossing point temperature of coal. International Journal of Mining Science and Technology (Formerly Mining Science and Technology (China)) 21:255–260

Yi J, Prybutok R (1996) A neural network model forecasting for prediction of daily maximum ozone concentration in an industrialised urban area. Environ Pollut 92:349–357

Yu H and Wilamowski BM (2010) Levenberg–Marquardt Training, Auburn University. www.eng.auburn.edu/~wilambm/pap/2011/K10149_C012.pdf. 2010. Accessed on 10.02.14