Data Article

Data on analysis of temperature inversion during spontaneous combustion of coal

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Abstract

Data in this article presents the characteristic parameters of spontaneous combustion of coal with different ranks, including lignite, long flame coal, and anthracite. The coal samples were tested by the temperature programmed method. The gas concentration data produced at different temperature points during the heating process are obtained. Through monitoring the spontaneous combustion of coal in a coal mine, the field data in goaf are obtained. Through processing on the data from the experiment and field, three gas indices were obtained, which include CO/CO2, Graham value and Alkane ratio. The data is made available for further use and for furthering the understanding of the key findings of the related research, such as the early warning for spontaneous combustion of coal. For more insight please see A method for evaluating the spontaneous combustion of coal by monitoring various gases (Guo et al., 2019).

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1. Data

The data shared in this paper include the gas data of coal samples acquired by the temperature programmed test, the field data from a coal mine with the spontaneous combustion of the coal seam, and processed data of the above data. The gas data (O₂, N₂, CO, CO₂, CH₄, C₂H₆, C₂H₄) of anthracite, lignite and two long-flame coal obtained through experimental tests, as shown in Tables 1–4. The field observation data is shown in Table 5, come from a goaf of coal seam where spontaneous combustion occurred. This coal seam belongs to a coal mine in Shaanxi province. What’s more, the three index parameter data (CO/CO₂, Graham value, chain alkane ratio) calculated from the index gas, as shown in Table 6 and Table 7.

2. Experimental design, materials and methods

2.1. Experimental design

2.1.1. Sample preparation

Select lignite, long flame coal, and anthracite, collect fresh exposed coal blocks in working face, crush them in air, sift out 200 g coal samples with particle size of 0–0.9 mm, 0.9–3 mm, 3–5 mm, 5–7 mm and 7–10 mm, mix them into 1000g samples, numbered 1–4#, and prepare for sealed storage test. The sample preparation process is shown in Fig. 1.
Table 1
Experimental data in lignite heating process.

| Temperature/°C | O₂/%  | N₂/%  | CO/ppm | CO₂/ppm | CH₄/ppm | C₂H₆/ppm | C₂H₄/ppm |
|---------------|-------|-------|--------|---------|---------|----------|----------|
| 30            | 20.42 | 79.36 | 14.83  | 988.67  | 6.08    | 0.88     | –        |
| 40            | 20.30 | 78.91 | 34.93  | 1397.20 | 9.11    | 1.24     | –        |
| 50            | 19.95 | 78.73 | 101.20 | 3264.52 | 11.11   | 1.46     | –        |
| 60            | 18.54 | 79.24 | 257.10 | 11178.26| 11.81   | 1.66     | –        |
| 70            | 16.78 | 80.31 | 454.40 | 18176.00| 4.90    | 1.14     | –        |
| 80            | 14.35 | 82.20 | 814.00 | 26258.07| 1.70    | 3.22     | –        |
| 90            | 14.11 | 82.82 | 1183.00| 30333.33| 1.96    | 5.62     | –        |
| 100           | 13.41 | 83.31 | 1042.00| 27421.05| 1.82    | 4.29     | –        |
| 110           | 12.89 | 82.82 | 11850.00| 96341.46| 2.54    | 7.45     | –        |
| 120           | 10.86 | 84.47 | 1725.00| 39204.55| 3.02    | 13.90    | –        |
| 130           | 4.92  | 88.83 | 2875.00| 55288.46| 4.64    | 23.30    | –        |
| 140           | 1.93  | 89.20 | 4746.00| 69794.12| 22.49   | 17.92    | –        |
| 150           | 1.27  | 88.38 | 7227.00| 83068.97| 5.48    | 20.62    | –        |
| 160           | 1.16  | 88.29 | 9431.00| 26258.07| 6.44    | 1.70     | 3.22     |
| 170           | 1.13  | 87.91 | 11850.00| 96341.46| 7.01    | 23.61    | –        |

Table 2
Experimental data in anthracite heating process.

| Temperature/°C | O₂/%  | N₂/%  | CO/ppm | CO₂/ppm | CH₄/ppm | C₂H₆/ppm | C₂H₄/ppm |
|---------------|-------|-------|--------|---------|---------|----------|----------|
| 30            | 20.64 | 78.61 | 6.64   | 2088.68 | 4.32    | 2.57     | –        |
| 40            | 20.79 | 78.40 | 7.91   | 1869.50 | 7.96    | 3.19     | –        |
| 50            | 20.83 | 78.22 | 8.89   | 1760.00 | 8.34    | 3.57     | –        |
| 60            | 20.53 | 78.22 | 21.90  | 2585.60 | 11.85   | 4.76     | –        |
| 70            | 20.10 | 78.38 | 50.80  | 4673.41 | 13.24   | 5.26     | –        |
| 80            | 19.44 | 79.22 | 94.90  | 6856.94 | 15.57   | 6.44     | –        |
| 90            | 18.82 | 79.51 | 159.90 | 9095.56 | 19.34   | 9.44     | –        |
| 100           | 18.74 | 79.47 | 216.40 | 7781.37 | 24.78   | 10.26    | –        |
| 110           | 18.81 | 80.52 | 310.00 | 5145.23 | 27.81   | 14.56    | 7.93     |
| 120           | 18.76 | 80.51 | 427.40 | 3810.97 | 34.16   | 18.72    | 9.78     |
| 130           | 18.37 | 80.61 | 628.10 | 3392.20 | 43.64   | 22.03    | 11.87    |
| 140           | 17.66 | 80.34 | 955.50 | 4562.17 | 56.59   | 28.89    | 14.83    |
| 150           | 15.37 | 82.29 | 1783.00| 8319.72 | 75.74   | 33.90    | 17.53    |
| 160           | 14.27 | 83.50 | 2477.00| 10250.79| 83.15   | 36.13    | 22.33    |
| 170           | 11.64 | 86.38 | 3732.00| 12462.02| 95.26   | 48.93    | 30.13    |

Table 3
Experimental data in long flame coal (1#) heating process.

| Temperature/°C | O₂/%  | N₂/%  | CO/ppm | CO₂/ppm | CH₄/ppm | C₂H₆/ppm | C₂H₄/ppm |
|---------------|-------|-------|--------|---------|---------|----------|----------|
| 30            | 20.85 | 78.66 | 6.50   | 664.15  | 10.71   | 4.03     | –        |
| 40            | 20.77 | 78.17 | 14.62  | 731.00  | 10.86   | 6.08     | –        |
| 50            | 20.65 | 78.40 | 38.12  | 953.00  | 10.89   | 13.65    | –        |
| 60            | 20.61 | 78.27 | 58.51  | 1244.89 | 12.21   | 16.68    | –        |
| 70            | 20.07 | 78.31 | 156.20 | 2947.17 | 13.37   | 18.00    | –        |
| 80            | 19.71 | 79.27 | 294.00 | 3500.00 | 14.58   | 20.86    | –        |
| 90            | 18.42 | 80.39 | 526.00 | 3867.65 | 14.69   | 23.35    | –        |
| 100           | 17.40 | 81.85 | 817.50 | 5413.91 | 15.98   | 23.87    | –        |
| 110           | 16.74 | 81.24 | 1174.00| 5870.00 | 16.17   | 24.81    | 1.03     |
| 120           | 16.47 | 82.10 | 1870.00| 9303.48 | 17.10   | 24.91    | 1.34     |
| 130           | 17.60 | 80.64 | 2106.00| 9360.00 | 18.22   | 29.39    | 3.83     |
| 140           | 16.18 | 80.72 | 3433.00| 13203.85| 34.58   | 31.23    | 9.24     |
| 150           | 11.43 | 84.11 | 9226.00| 25310.69| 83.14   | 33.65    | 13.38    |
| 160           | 10.39 | 85.07 | 11450.00| 24361.70| 123.15  | 34.81    | 16.33    |
| 170           | 9.69  | 85.51 | 13950.00| 27493.64| 155.80  | 36.22    | 24.25    |
Table 4
Experimental data in long flame coal (2#) heating process.

| Temperature/°c | O₂/%  | N₂/%  | CO/ppm | CO₂/ppm | CH₄/ppm | C₂H₆/ppm | C₂H₄/ppm |
|----------------|-------|-------|--------|---------|---------|----------|----------|
| 30             | 20.78 | 78.73 | 3.25   | 160.29  | 2.37    | 1.03     | –        |
| 40             | 20.30 | 79.07 | 11.86  | 966.80  | 2.39    | 1.35     | –        |
| 50             | 20.64 | 78.45 | 17.18  | 580.60  | 2.47    | 2.31     | –        |
| 60             | 20.09 | 78.76 | 54.32  | 1522.42 | 2.58    | 2.69     | –        |
| 70             | 20.21 | 79.21 | 83.07  | 1560.59 | 2.63    | 3.66     | –        |
| 80             | 19.65 | 79.33 | 187.20 | 3657.68 | 2.72    | 4.06     | –        |
| 90             | 18.30 | 80.02 | 370.20 | 6576.66 | 3.05    | 4.10     | –        |
| 100            | 17.46 | 82.09 | 491.90 | 7264.81 | 3.42    | 4.24     | 1.55     |
| 110            | 16.41 | 82.70 | 809.80 | 6739.91 | 4.57    | 4.63     | 3.09     |
| 120            | 12.47 | 85.08 | 1819.00| 12781.96| 8.51    | 6.47     | 4.91     |
| 130            | 10.57 | 85.75 | 2859.00| 14785.17| 13.38   | 10.45    | 9.25     |
| 140            | 7.39  | 88.19 | 4647.00| 25214.32| 25.80   | 15.59    | 14.30    |
| 150            | 7.24  | 88.13 | 6432.00| 31400.12| 42.99   | 21.59    | 24.08    |
| 160            | 5.14  | 88.58 | 9150.00| 41719.86| 86.00   | 23.94    | 32.88    |
| 170            | 4.56  | 89.15 | 11350.00| 47944.92| 121.50  | 25.64    | 36.77    |

Table 5
The field observation data.

| Time/d | O₂/%  | N₂/%  | CO/ppm | CO₂/%  | CH₄/%  | C₂H₆/%  |
|--------|-------|-------|--------|--------|--------|---------|
| 1      | 14.37 | 74.33 | 0.00   | 0.22   | 8.02   | 3.01    |
| 2      | 14.26 | 71.20 | 0.00   | 0.24   | 9.70   | 4.02    |
| 3      | 14.37 | 71.65 | 0.00   | 0.16   | 8.63   | 4.94    |
| 4      | 11.98 | 73.78 | 0.00   | 0.38   | 8.20   | 3.82    |
| 5      | 11.59 | 76.21 | 0.01   | 0.33   | 6.87   | 4.36    |
| 6      | 12.68 | 78.01 | 0.01   | 0.31   | 4.84   | 3.57    |
| 7      | 13.87 | 77.41 | 0.01   | 0.29   | 4.35   | 3.60    |
| 8      | 12.93 | 76.97 | 0.01   | 0.37   | 4.95   | 4.03    |
| 9      | 14.30 | 74.40 | 0.01   | 0.24   | 5.68   | 5.27    |
| 10     | 14.52 | 74.65 | 0.01   | 0.22   | 5.44   | 5.14    |
| 11     | 14.73 | 77.80 | 0.01   | 0.19   | 2.82   | 3.56    |
| 12     | 14.25 | 75.70 | 0.01   | 0.22   | 3.98   | 4.82    |
| 13     | 14.56 | 76.02 | 0.01   | 0.20   | 4.07   | 5.04    |
| 14     | 14.32 | 77.38 | 0.01   | 0.24   | 4.27   | 3.64    |
| 15     | 13.44 | 77.10 | 0.01   | 0.25   | 4.61   | 4.42    |
| 16     | 15.13 | 76.09 | 0.01   | 0.19   | 4.14   | 4.12    |
| 17     | 13.35 | 77.94 | 0.01   | 0.22   | 4.02   | 3.85    |
| 18     | 14.01 | 77.11 | 0.01   | 0.24   | 4.24   | 4.29    |
| 19     | 12.61 | 78.17 | 0.01   | 0.25   | 4.24   | 3.66    |
| 20     | 11.67 | 78.01 | 0.01   | 0.26   | 4.49   | 5.27    |
| 21     | 11.50 | 80.10 | 0.01   | 0.32   | 4.14   | 3.70    |
| 22     | 12.75 | 76.73 | 0.01   | 0.25   | 4.57   | 5.38    |
| 23     | 12.05 | 76.49 | 0.01   | 0.24   | 5.18   | 5.78    |
| 24     | 12.92 | 76.06 | 0.01   | 0.23   | 5.13   | 5.57    |
| 25     | 13.24 | 77.38 | 0.01   | 0.24   | 3.88   | 4.56    |
| 26     | 13.61 | 77.60 | 0.01   | 0.23   | 3.38   | 4.80    |
| 27     | 12.51 | 78.22 | 0.01   | 0.29   | 3.85   | 4.84    |
| 28     | 10.33 | 79.61 | 0.01   | 0.37   | 4.08   | 4.51    |
| 29     | 11.75 | 80.57 | 0.01   | 0.35   | 3.59   | 3.49    |
| 30     | 12.56 | 78.73 | 0.01   | 0.27   | 3.95   | 4.32    |
| 31     | 12.64 | 79.38 | 0.01   | 0.27   | 3.86   | 3.66    |
| 32     | 12.78 | 78.18 | 0.01   | 0.23   | 3.75   | 4.90    |
| 33     | 10.46 | 80.05 | 0.01   | 0.35   | 4.19   | 2.91    |
| 34     | 11.17 | 81.60 | 0.01   | 0.27   | 3.58   | 3.20    |
| 35     | 11.03 | 81.89 | 0.01   | 0.45   | 3.58   | 2.53    |
### Table 6
Calculations results of gas index data for different coal samples.

| Temperature/°C | Lignite | Anthracite | Long flame coal (1#) | Long flame coal (2#) |
|----------------|---------|------------|----------------------|----------------------|
|                | CO/CO₂  | Graham Alkane ratio | CO/CO₂  | Graham Alkane ratio | CO/CO₂  | Graham Alkane ratio | CO/CO₂  | Graham Alkane ratio |
| 30             | 0.015   | 0.255      | 0.097               | 0.010               | 0.433   | 0.249               | 0.020   | 0.150               | 0.429   |
| 40             | 0.025   | 0.499      | 0.117               | 0.020               | 0.636   | 0.560               | 0.012   | 0.168               | 0.545   |
| 50             | 0.031   | 0.966      | 0.160               | 0.040               | 1.089   | 0.929               | 0.030   | 0.481               | 0.898   |
| 60             | 0.023   | 1.047      | 0.146               | 0.047               | 1.500   | 1.144               | 0.036   | 0.598               | 1.020   |
| 70             | 0.025   | 1.077      | 0.126               | 0.053               | 1.680   | 1.463               | 0.053   | 1.052               | 1.347   |
| 80             | 0.031   | 1.223      | 0.182               | 0.084               | 2.279   | 1.916               | 0.051   | 1.387               | 1.331   |
| 90             | 0.037   | 1.486      | 0.194               | 0.136               | 2.039   | 2.180               | 0.056   | 1.370               | 1.201   |
| 100            | 0.038   | 1.373      | 0.186               | 0.151               | 2.271   | 1.955               | 0.068   | 1.389               | 0.928   |
| 110            | 0.039   | 1.664      | 0.147               | 0.200               | 2.756   | 1.553               | 0.120   | 1.766               | 0.544   |
| 120            | 0.044   | 1.701      | 0.144               | 0.201               | 4.129   | 1.457               | 0.142   | 2.132               | 0.484   |
| 130            | 0.052   | 1.788      | 0.113               | 0.225               | 6.194   | 1.613               | 0.164   | 2.740               | 0.405   |
| 140            | 0.068   | 2.489      | 0.074               | 0.260               | 7.122   | 1.271               | 0.184   | 3.414               | 0.363   |
| 150            | 0.087   | 3.663      | 0.064               | 0.365               | 9.645   | 1.045               | 0.205   | 4.675               | 0.251   |
| 160            | 0.103   | 4.754      | 0.065               | 0.470               | 10.792  | 0.283               | 0.219   | 5.770               | 0.197   |
| 170            | 0.123   | 5.965      | 0.064               | 0.507               | 12.330  | 0.232               | 0.237   | 6.902               | 0.175   |

### Table 7
Calculation results of gas index data for field monitoring.

| Time/d | CO/CO₂  | 10 × Graham Alkane ratio | Alkane ratio | Time/d | CO/CO₂  | 10 × Graham Alkane ratio | Alkane ratio |
|--------|---------|--------------------------|--------------|--------|---------|--------------------------|--------------|
| 1      | 0.014   | 0.467                    | 0.375        | 19     | 0.040   | 1.216                    | 0.863        |
| 2      | 0.015   | 0.519                    | 0.415        | 20     | 0.042   | 1.168                    | 1.173        |
| 3      | 0.024   | 0.573                    | 0.572        | 21     | 0.036   | 1.200                    | 0.895        |
| 4      | 0.012   | 0.521                    | 0.466        | 22     | 0.045   | 1.394                    | 1.177        |
| 5      | 0.016   | 0.574                    | 0.634        | 23     | 0.048   | 1.318                    | 1.115        |
| 6      | 0.019   | 0.709                    | 0.738        | 24     | 0.053   | 1.485                    | 1.085        |
| 7      | 0.023   | 0.939                    | 0.827        | 25     | 0.048   | 1.507                    | 1.177        |
| 8      | 0.020   | 0.929                    | 0.814        | 26     | 0.051   | 1.611                    | 1.422        |
| 9      | 0.035   | 1.225                    | 0.927        | 27     | 0.042   | 1.425                    | 1.256        |
| 10     | 0.041   | 1.389                    | 0.944        | 28     | 0.033   | 1.153                    | 1.103        |
| 11     | 0.053   | 1.562                    | 1.265        | 29     | 0.034   | 1.265                    | 0.572        |
| 12     | 0.054   | 1.734                    | 1.213        | 30     | 0.043   | 1.363                    | 1.094        |
| 13     | 0.056   | 1.738                    | 1.238        | 31     | 0.044   | 1.399                    | 0.949        |
| 14     | 0.042   | 1.497                    | 0.854        | 32     | 0.047   | 1.338                    | 1.307        |
| 15     | 0.041   | 1.348                    | 0.958        | 33     | 0.032   | 1.063                    | 0.694        |
| 16     | 0.051   | 1.636                    | 0.994        | 34     | 0.043   | 1.201                    | 0.896        |
| 17     | 0.039   | 1.137                    | 0.958        | 35     | 0.026   | 1.183                    | 0.706        |
| 18     | 0.039   | 1.330                    | 1.011        |        |         |                          |              |

**Fig. 1.** A flow chart summarizing coal sample processing process.
2.1.2. Experimental test method

A temperature programmed test system for spontaneous combustion of coal in air bath is used in the experiment [2–4]. The structure of the system is shown in Fig. 2. Using this experimental device, coal samples are loaded into a cylindrical special steel coal sample tank with a diameter of 10 cm at the bottom and a height of 25 cm. As shown in Fig. 2, the experiment begins after sealing. Using an air pump or gas cylinder as a gas source, the air is supplied to a coal sample tank with 120 ml/min air flow. Air flows through a glass rotor flowmeter and gas conveying copper pipe, preheated by the heating box, and then passes through the bottom of the coal sample tank to the coal sample. After 30 minutes of venting air, the gas samples were collected at the rate of 0.3 °C/min and then analyzed by the SP-2120 gas chromatograph. The component data of gas products at different temperature points were obtained.

2.2. Data analysis

When the experimental data and field data are obtained, the biggest influence factor is the difference in air volume [5,6], so there are significant differences in the data results. In the analysis of the results, it is necessary to eliminate the dilution effect of air flow on the gas as far as possible. The gas index can satisfy this condition very well [7]. In addition, the mechanism of producing index gas in the coal oxidation process is different, CO and a lot of CO2 are produced. It is produced by the oxidation reaction between coal and oxygen. Some coal seams contain a part of CO2, CH4 and C2H6 gas, which will be resolved at low temperatures. There is generally no C2H4 in coal seams. C2H4 gas is produced mainly by cracking, so different gas means the reaction function represented by the standard is also different [8–10]. CO/CO2 can better reflect the intensity of oxidation, Graham value (G = ΔCO/ΔO2) can reflect the relationship between oxygen consumption and CO formation, and alkane ratio can reflect the intensity of coal pyrolysis [11]. By calculating the experimental and field data, the gas index data are obtained as shown in Tables 6 and 7.

2.3. Inversion method of coal temperature

By calculating the results of experimental data and field data, the results can be well corresponded. The natural ignition trend of the coal seam is qualitatively analyzed by selecting standard gas through

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Fig. 2. The temperature programmed experimental apparatus.
experiments, and the degree of spontaneous combustion of the coal seam is quantitatively analyzed by gas index. The development law of spontaneous combustion of the coal seam in mine is predicted by combining the two kind of indexes [1]. The forecasting idea is shown in Fig. 3.

As shown in Fig. 3, firstly using a single indicator to qualitatively determine the potential for spontaneous combustion. The CO volume fraction is employed to determine the likelihood of spontaneous combustion. Due to C$_2$H$_4$ appeared above approximately 110 °C, so its volume fraction is also assessed to qualitatively evaluate the probability of spontaneous combustion. Secondly, using the gas ratio to determine the probability of spontaneous combustion. The CO/CO$_2$ ratio, Graham coefficient, and alkyl chain ratio are all determined via on-site measurements. Based on correlations derived from experimental testing, the above ratios are used to find the coal temperature. A comprehensive analysis of single gases such as CO and C$_2$H$_4$ as well as gas ratios is employed to calculate the coal temperature. The average values of the on-site indicators are calculated so as to obtain the average coal temperature at the site. The prediction accuracy and confidence intervals are set to the desired values. The degree of confidence for each temperature value obtained from the above process is calculated. An application of these data and this early warning for spontaneous combustion of coal can be found in Ref. [1].

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**Conflict of interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
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