**Supplementary Material**

1. **The oxidation kinetics experiment**

The oxidation kinetics experiment system in section 3.2.2 was designed according to AQ/T 1068-2008 “The test method of oxidation kinetics for the propensity of coal to spontaneous combustion.” And, experiment was implemented on the basis of AQ/T 1019-2006 “The method of gas chromatography analysis and index optimization for mark gases of spontaneous combustion of coal stratum.” Results are shown in Table 1.

Table 1 Gas concentrations of raw coal during programmed temperature

|  |  |  |  |
| --- | --- | --- | --- |
| Temperature/oC | O2/% | CO/10-6 | CO2/10-6 |
| 30 | 21.09 (±0.01) | 0 | 0 |
| 40 | 21.08 (±0.01) | 0 | 27 (±3) |
| 50 | 21.07 (±0.01) | 0 | 62 (±4) |
| 60 | 21.05 (±0.02) | 6 (±2) | 106 (±5) |
| 70 | 20.99 (±0.02) | 13 (±2) | 161 (±5) |
| 80 | 20.89(±0.03) | 23 (±3) | 213 (±6) |
| 90 | 20.77(±0.04) | 38 (±4) | 418 (±9) |
| 100 | 20.62(±0.06) | 54 (±6) | 599 (±14) |

On the basis of accurate operation, the error is reasonable. The average of the gas concentrations is used to calculate the consumption and the generation rate.

1. **The calculation process of the thermal effects**

**1**: The shortest spontaneous combustion period is the sum of the heating time of four heating intervals, which are respectively raw-40 oC, 40-60 oC, 60-80 oC, 80-100 oC.

**2**: $t\_{t\_{1}- t\_{2}}$*-*heating time from t1 oC to t2 oC*.* $∆T$*-*interval temperature (20 oC)*.* $ρ\_{c}$*-*density of loose coal, g·cm-3. $c\_{c}$-specific heat of loose coal, J·g-1·°C -1. $q\_{max}(T)$-the maximum heat release intensity, J·cm-3·s-1

$ρ\_{c} $*and* $c\_{c}$ were obtained from the basic data in Table 1. The pore and air specific heat capacity were also taken into account.

**3**: $V\_{O\_{2}}$-consumption rate of O2. $V\_{CO}$$V\_{CO}$-generation rate of CO. $V\_{CO\_{2}}$$V\_{CO\_{2}}$-generation rate of CO2. $∆H\_{two}^{''}$$∆H\_{two}^{''}$-average thermal effect from reactants to intermediates (O=C and O=C-O) according to reaction mechanism. $∆H\_{CO}^{''}$$∆H\_{CO}^{''}$-average thermal effect of generating CO. $∆H\_{CO\_{2}}^{''}$$∆H\_{CO\_{2}}^{''}$-average thermal effect of generating CO2.

The numbers in brackets represent reaction lines involving generation of CO, CO2 and second step reaction.

**4**: Because CO, CO2 and intermediates (O=C and O=C-O) are generated by different reaction lines, the average thermal effects are calculated according to the reaction ratio and thermal effect of different lines.

**5**: m:n-the reaction ratio obtained by infrared and XPS analysis in oxidation process. $∆H\_{two}^{1/2/3/4/5/6}$$∆H\_{two}^{1/2/3/4/5/6}$-thermal effect of the generated intermediates (O=C and O=C-O) in reaction line 1/2/3/4/5/6; $∆H\_{CO}^{1/2/4/5/6}$$∆H\_{CO}^{1/2/4/5/6}$-thermal effect of the generated CO in reaction line 1/2/4/5/6; $∆H\_{CO\_{2}}^{1/2/3/4}$$∆H\_{CO\_{2}}^{1/2/3/4}$-thermal effect of the generated CO2 in reaction line 1/2/3/4.