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The Influence of Composition on Calorific Value and the Adiabatic Flame Temperature of Coal

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Abstract: A quantitative analysis was conducted on the factors influencing the calorific value and adiabatic combustion temperature of coal. The analysis revealed that the rank correlation coefficients between the calorific value and the carbon, hydrogen, and sulfur contents in coal were 0.886, 0.214, and 0.27, respectively. To reduce dimensionality, the Car, Har, and Sar components of coal were integrated into a single variable, resulting in a regression model for the calorific value and the integrated variable. The model's coefficient of determination was $R^2 = 0.8619$, the adjusted coefficient of determination $A.R^2 = 0.8587$, explaining 85.87% of the variation in the calorific value. Based on combustion principles, a nonlinear regression was performed for the adiabatic combustion temperature. The standard errors of the model parameters were 0.002564 and 0.1655, respectively. The mean relative deviation between the measured and predicted values was 7.79%, with a standard deviation of 19.74°C for the coal samples. The average relative residual was 7.79, with a median of 6.66. The residual distribution exhibited right skewness, indicating potential for further improvement.

Keywords: Pulverized coal; Regression analysis; Lower calorific value; Adiabatic flame temperature

1. Introduction

The design of pulverized coal boilers is a complex systems engineering task involving combustion, heat transfer, and fluid dynamics. Its objective is to ensure the efficient conversion of chemical energy in coal into steam thermal energy while maintaining safety and reliability. Combustion calculation serves as the starting point for boiler design and constitutes a critical auxiliary calculation[1]. Based on fundamental data such as elemental analysis, calorific value, and ash characteristics of coal, combustion calculations apply the first and second laws of thermodynamics to determine key parameters including air consumption, flue gas generation, and adiabatic combustion temperature under complete combustion conditions. These results provide essential inputs for subsequent furnace thermal calculations, convective heating surface thermal calculations, and the design of the air and flue gas system. The determination of air consumption relies on the elemental composition of the coal. Under the assumption of complete combustion, both the theoretical air requirement and the actual air consumption are calculated[2]. The actual air consumption is determined by incorporating the excess air coefficient—dictated by the combustion system and heating surface arrangement—alongside the theoretical air requirement[3]. Flue gas calculations encompass both the volume and composition of the flue gas, particularly the proportion of triatomic gases such as CO_2, H_2O, SO_2, and particulate ash. These calculations provide a basis for the selection of induced draft fans, as well as the design of flue ducts and chimneys. Furthermore, flue gas data serve as fundamental inputs for determining the required airflow for dust collectors, reagent consumption in desulfurization systems, catalyst usage in denitrification systems, and preventing low-temperature corrosion in air preheaters[4].

The calorific value and adiabatic combustion temperature of coal are two key parameters that reflect its energy conversion potential and combustion state, exhibiting strict intrinsic relationships and interaction mechanisms with the main components of coal. Considering that calorific value is associated with combustible components such as carbon and hydrogen, this study conducted correlation and regression analyses on coal commonly used in thermal power plants in China to quantitatively understand the influence of combustible components on coal calorific value. The adiabatic combustion temperature, a critical parameter for furnace thermal calculations, depends on the coal's calorific value and flue gas characteristics, including flue gas volume, composition, and fly ash content. To quantitatively identify the main influencing factors of adiabatic combustion temperature, a multiple nonlinear regression analysis was performed.

2. Experimental

The test coal samples cover anthracite, lean coal, bituminous coal, and lignite. Elemental analysis of coal was performed using an Elementar vario MICRO cube elemental analyzer, calibrated with acetanilide prior to each analysis. Approximately 5 mg of coal sample was weighed and introduced into the high-temperature combustion tube via an automatic sampler. The outlet gas mixture was purified through a reduction tube and adsorbent, separated by a chromatographic column, and detected by a thermal conductivity detector (TCD) to determine the content of elements such as C, H, N, and S in the coal. Moisture and ash content were measured according to GB/T 483-2007, with the drying oven temperature set at 102–105°C and sample ashing conducted in a muffle furnace at 800±20°C. The lower heating value of coal was determined using an oxygen bomb calorimeter, and the calorimeter's heat capacity was calibrated with benzoic acid. The elemental analysis results and lower heating values of each coal sample are presented in Table 1.

Table 1. Ultimate Analysis and Net Calorific Value of Coal Samples

Samples	Car [%]	Har [%]	Oar [%]	Nar [%]	Sar [%]	Mar [%]	Aar [%]	Qar,net [kJ/kg]
WY-1	67.11	2.63	2.6	1.07	1.55	8.4	16.64	25288
WY-2	56.96	2.55	4.3	0.97	0.7	3.82	30.62	23488
WY-3	66.99	2.15	2.38	0.75	0.28	10.21	17.24	24279
WY-4	62.88	1.82	2.4	0.64	1.36	11.37	19.53	23697
WY-5	62	2.38	1.65	0.77	0.35	14.17	18.68	22366
WY-6	57.95	2.24	2.63	0.7	0.26	7.18	29.04	20984
WY-7	54.37	2.04	1.73	0.66	3.58	9.2	28.42	22780
WY-8	55.81	2.43	3.97	0.86	3.96	10.44	22.43	24254
WY-9	54.37	2.56	2.75	0.88	3.64	11.33	24.46	23287
PM-1	70.8	3.12	2.46	0.94	1.53	5.42	15.73	27470
PM-1	70.05	3.15	2.26	0.96	1.62	5.99	15.97	25660
PM-1	56.31	2.88	1.56	0.89	2.83	6.07	29.46	22739
PM-1	65.54	2.84	2.34	0.1	3.37	4.91	20.9	25636
PM-1	70.54	2.91	1.65	1.08	0.31	7.8	15.71	26205
PM-1	64.55	3.2	2.08	1.14	1.12	6.14	21.77	24593
PM-1	56.67	2.89	2.83	0.64	5.3	4.9	26.77	22358

3. Results and Discussion

3.1. Influencing Factors of Calorific Value

Calorific value is the most important technical property of steam coal, and its magnitude is related to the combustible content in the coal. In current combustion calculations for boiler thermal design, carbon, hydrogen, oxygen, nitrogen, and sulfur in coal are all considered combustible components. However, in actual combustion, the calorific value fundamentally depends on the content of elements such as carbon, hydrogen, and sulfur. To quantitatively analyze the influence of these combustible components on calorific value, a rank correlation analysis was conducted between the calorific value and the contents of carbon, hydrogen, sulfur, and other elements in the coal, as shown in Figures 1–3.

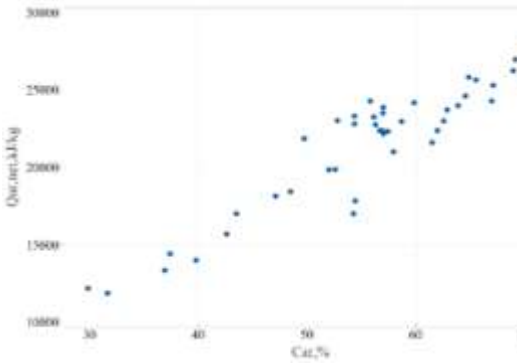


Figure 1. Monotonic Relationship Between Carbon Content and Calorific Value.

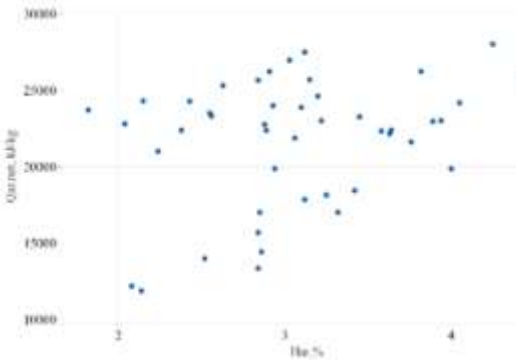


Figure 2. Monotonic Relationship Between Hydrogen Content and Calorific Value.

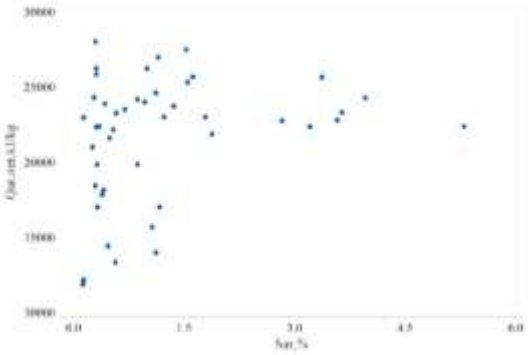


Figure 3. Monotonic Relationship Between Sulphur Content and Calorific Value.

As shown in Figure 1, there exists a strong positive correlation between carbon content and calorific value, with a rank correlation coefficient of 0.886. Figure 2 and Figure 2, however, indicate only weak positive correlations between the content of elements such as hydrogen and sulfur in coal and the calorific value, with rank correlation coefficients of 0.214 and 0.27, respectively. At first glance, this suggests that the calorific value is primarily determined by the carbon content in coal, while hydrogen and sulfur have little influence. However, this conclusion is clearly inconsistent with factual thermodynamic principles and warrants careful analysis. From a causal perspective, the calorific value of coal

depends not only on the content of elements such as carbon, hydrogen, and sulfur but also on their respective heat release upon oxidation. Under standard thermochemical conditions, the combustion enthalpy of graphite is -393.8 kJ/mol, that of hydrogen is -285.8 kJ/mol, and that of elemental sulfur is -296.8 kJ/mol. The calorific contributions of these three elements are of the same order of magnitude. Therefore, it is reasonable to expect that the contents of carbon, hydrogen, and sulfur in coal should all exhibit strong positive correlations with the calorific value. The weak correlations observed in Fig.2 and Fig.3 can be attributed to the fact that the calorific value of coal is not solely determined by the inherent energy of combustible elements but also by their relative abundances. In all the coal samples studied, the average and median carbon contents are 56.23% and 56.96%, respectively, while the average and median hydrogen contents are 3.06% and 3.03%, and those of sulfur are 1.21% and 0.87%. Compared to hydrogen and sulfur, the carbon content is significantly higher. Coupled with the higher standard combustion enthalpy of carbon, this dominance diminishes the apparent statistical influence of hydrogen and sulfur on the calorific value, resulting in the observed weak correlations. Hence, it is not justified to simply ignore the effects of hydrogen and sulfur content on the calorific value. To quantitatively understand the influence of carbon, hydrogen, and sulfur content in coal on the calorific value, a regression analysis was performed.

Considering that the calorific value of coal is primarily determined by the content of elements such as carbon, hydrogen, and sulfur, the regression process began by integrating these elemental contents into a single composite variable. This approach was adopted to reduce the dimensionality of independent variables in the regression analysis and simplify the modeling procedure. The integration was performed based on the following principle: it was assumed that carbon in coal exists in the form of graphite, hydrogen as hydrogen gas, and sulfur as elemental sulfur. Following this rule and incorporating the standard combustion enthalpies of graphite, hydrogen gas, and elemental sulfur, the composite variable X was derived as follows:

$$X=10\left(\frac{C_{ar}}{MW_C}\Delta H^0_{c,C}+\frac{H_{ar}}{MW_{H_2}}\Delta H^0_{c,H_2}+\frac{S_{ar}}{MW_S}\Delta H^0_{c,S}\right), kJ/kg \quad (1)$$

In the above equation, MWC, MWH_2, and MWS represent the molecular weights of graphite, hydrogen, and sulfur, respectively, while $\Delta H°c,C$, $\Delta H°c,H_2$, and $\Delta H°c,S$ denote the standard combustion enthalpies of graphite, hydrogen, and elemental sulfur.

Then, a simple linear regression was performed between variable X and the calorific value of coal, yielding the following regression model:

$$Q_{ar,net}=-1798+1.02X, kJ/kg \quad (2)$$

The regression model (2) has a coefficient of determination (R^2) of 0.8619 and an adjusted R^2 of 0.8587, with a p-value of 0 for the significance test. This indicates that the model possesses strong explanatory power. The composite variable X, which integrates the three independent variables Car, Har, and Sar, collectively explains 85.87% of the variance in the calorific value of coal. The model demonstrates a high goodness of fit and strong predictive capability, with detailed results illustrated in the figure below:

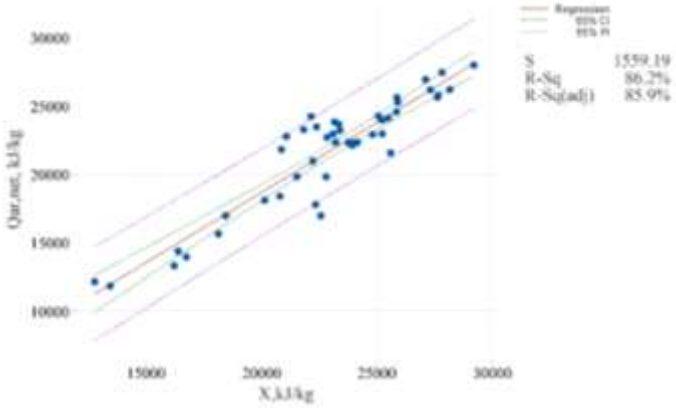


Figure 4. The regression equation, confidence interval, and prediction interval (at a 95% confidence level) for Regression Model (2)

As shown in Figure 4, among all coal samples, the measured values of three samples fall outside the prediction interval, accounting for 2.7% of the total. This meets the 5% threshold requirement, confirming that Regression Model (2) is valid and reliable.

3.2. Influencing Factors of the adiabatic flame temperature

The adiabatic flame temperature is a critical parameter in furnace thermal calculations, defined as the maximum temperature to which the flue gas is heated by combustion under adiabatic conditions, utilizing the calorific value of coal and the sensible heat of preheated air. Under these conditions, the combustion process of coal and air is isoenthalpic. Based on this principle, the functional form of the nonlinear regression relationship between the adiabatic flame temperature and the coal's calorific value, air preheat temperature, and flue gas volume is constructed as follows:

$$T_a=\frac{aQ_{ar,net}+bT_{air}}{V_y} \quad (3)$$

The variables in the equation above are defined as follows: T_a is the adiabatic flame temperature, T_{air} is the air preheating temperature, Vy is the theoretical flue gas volume, with a and b being the parameters to be determined. Based on the form of Equation (3), a nonlinear regression analysis was conducted, resulting in the following specific equation:

$$T_a=\frac{0.5808Q_{ar,net}+0.3023T_{air}}{V_y} \quad (4)$$

The regression results indicate parameter values of a= 0.5808 (SE = 0.002564, 95% CI [0.5756, 0.5860]) and b = 0.3023 (SE = 0.1655, 95% CI [–0.0313, 0.630]).

Based on regression equation (4), the relatively large standard error of parameter b indicates that the air preheat temperature used for the tested coal samples has a limited influence on the model. The coal samples in this study cover anthracite, lean coal, bituminous coal, and lignite. Given the critical importance of ignition characteristics and combustion stability in boiler design, different air preheat temperatures were applied to different coal samples. The specific air preheat temperatures used for each sample in the study are shown in Figure.5.

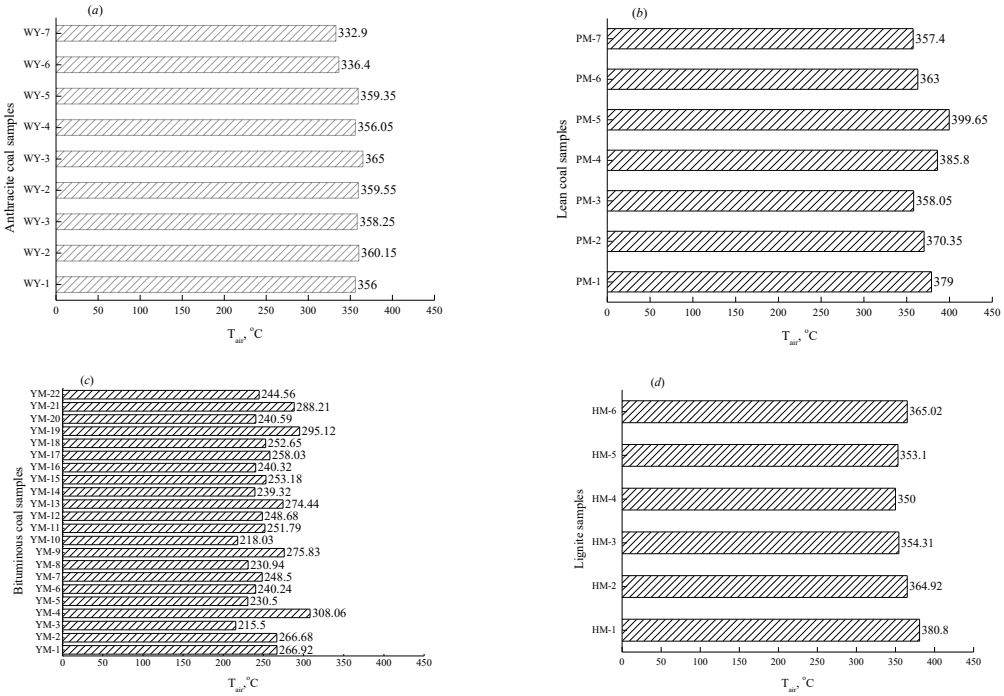


Figure 5. Air Preheating Temperatures Required for Combustion of Coal Samples.

(a) Anthracite; (b) Lean Coal; (c) Bituminous Coal; (d) Lignite

In Fig.5, the air preheating temperatures for anthracite, lean coal, and bituminous coal are determined based on the dry ash-free volatile matter content of the coal, with values of 300–400°C for anthracite and lean coal, and 250–300°C for bituminous coal. For lignite, the preheating temperature is set according to its moisture content, ranging from 300 to 400°C. Overall, the heat input contributed by air preheating accounts for 6.51–12.61% of the total heat input into the furnace, exerting a limited influence on the adiabatic flame temperature. This explains the relatively large standard error of parameter b in regression model (4).

To reasonably evaluate the validity of the nonlinear regression model (4), Figure 6 presents the measured values of the adiabatic flame temperature alongside the model-predicted values:

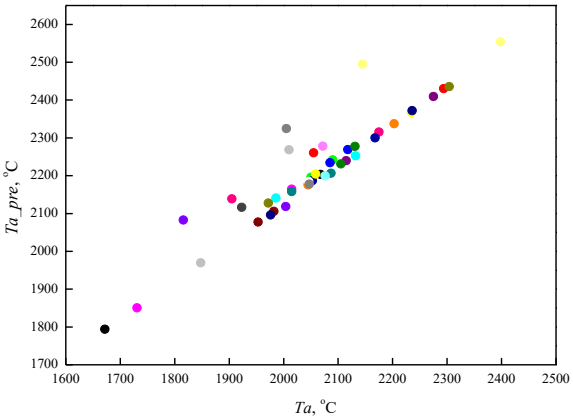


Figure 6. Fitting Curve of Regression Equation (4).

As shown in Fig.6, the measured values of the adiabatic flame temperature generally align along a straight line with the predicted values. The mean relative deviation between the measured and predicted values is 7.79%, with a standard deviation of 19.74°C across the coal samples. However, significant discrepancies are observed for seven individual samples. To further analyze the overall predictive capability of Model (4), Fig.7 presents the regression performance plot of the model.

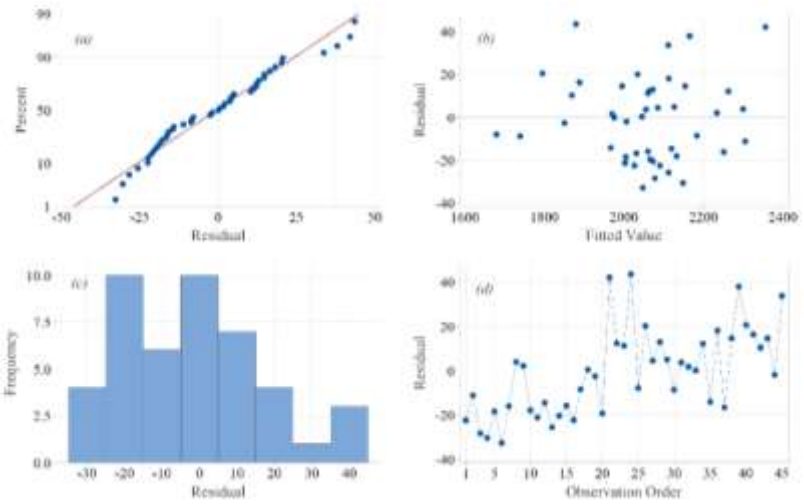


Figure 7. Regression Performance of Equation (4).

Figure 7(b) displays the fitted residual plot of Model (4). It can be observed that the sample data points are distributed relatively evenly on both sides of the zero residual line, indicating that Model (4) provides sufficient accuracy for predicting the adiabatic flame temperature and meets the requirements for engineering design. Figure 7(a) shows the normal probability plot of the residuals of Model (4). The data points largely follow the reference line, with those in the central region particularly close to the line and no clear systematic deviation. However, an upward curvature is noticeable in the middle segment of the probability distribution. Calculations show that the mean relative residual between measured and predicted values is 7.79, with a median of 6.66, and the residual distribution exhibits right skewness. Furthermore, this observation is supported by the residual histogram in Figure 7(c) and the observed value order plot of residuals in Figure 7(d), collectively suggesting that there remains room for further improvement in Model (4).

4. Conclusion

1) A strong positive correlation was observed between the calorific value and the carbon content in coal, with a rank correlation coefficient of 0.886, while weaker positive correlations were found with hydrogen and sulfur contents, having rank correlation coefficients of 0.214 and 0.27, respectively.

2) By integrating Car, Har, and Sar in coal into a single composite variable, a regression model between the calorific value and the integrated variable was established. The model achieved a coefficient of determination (R^2) of 0.8619, an adjusted R^2 of 0.8587, and a p-value of 0 for the significance test. These results indicate strong explanatory power, accounting for 85.87% of the variation in the calorific value.

3) Based on combustion principles, a nonlinear regression was performed for the adiabatic flame temperature. The standard errors of the model parameters were 0.002564 and 0.1655, with 95% confidence intervals of [0.5756, 0.5860] and [-0.0313, 0.630], respectively. The mean relative deviation between the measured and predicted values was 7.79%, and the standard deviation of the coal samples was 19.74°C.

4) For the nonlinear regression model of the adiabatic flame temperature, the mean relative residual was 7.79, with a median of 6.66. The residual distribution exhibited right skewness, indicating potential for further improvement in the model.

Conflicts of Interest

The authors declare that they have no conflict of interest.

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