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Research Article

APPLICATION OF GOLD SECTION METHOD IN CALCULATING THE PALEOGEOLOGIC TIME OF THE COAL THERMAL KINETIC EQUATION

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ABSTRACT

Knowing the vitrinite reflectance and the paleogeologic temperature, the iterative algorithms can be used to solve the paleogeologic time in the coal thermal dynamics equation. The required paleogeologic time is selected as the iterative variable to establish a relationship that can be iterative. The iterative process is controlled with the difference of the iterative values to limit the loop times. The relationship between the new iteration value and the previous iteration value was optimized with the gold section value of 0.618.The simplicity and effectiveness of the calculations is illustrated with 5 examples in the Carboniferous, Jurassic, and Cretaceous, respectively.

Keywords: coal thermal dynamics equation; paleogeologic time; iterative algorithm; gold section method.

INTRODUCTION

Coalification is the physical and chemical structure of peat. Under the action of temperature, pressure, time and other factors, it undergoes the change of physical and chemical properties of lignite, sub bituminous coal and bituminous coal, and finally becomes anthracite. It is also called coal metamorphism. The influence and control of two external factors (temperature and time) on coalification is comprehensive and crucial. Vitrinite reflectance is often used to express the degree of coal metamorphism in geological research. Wu Chonglong and Yang Qi, based on the general principles of geothermal and chemical dynamics, referring to the Bostick curve and the measured data of Meso Cenozoic in China, adopt the method of double regression to establish the three variable empirical formula of temperature-time-reflectance [1-5], which quantitatively represents the thermal dynamics of coal metamorphism. According to the three variable equation of temperature-time-reflectance [6-8], some articles discuss the difference of thermal dynamics between natural metamorphic coalification and artificial upgrading coalification. In addition, the paper calculates the minimum metamorphic temperature of coal seam with known absolute age and vitrinite reflectance. Some articles also calculate the maximum metamorphic limit of known absolute age and metamorphic temperature, that is, the reflectance of coal seam vitrinite. It is also quantitatively explained that the influence of increasing temperature on improving the degree of coal metamorphism is greater than that of prolonging time. These examples of calculating reflectance through time and temperature, calculating temperature through time and reflectance, and calculating the critical temperature of lignite or long flame coal prove that the empirical formula of temperature time reflectance can explain coal metamorphism to a certain extent, but it belongs to an equation with accurate solution from a mathematical point of view. That is, all independent variables (known quantities) are on the right side of the equation, and the right side does not contain dependent variables.

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The dependent variable (quantity to be solved) is only on the left of the equation, and there is only one mathematical operation. Therefore, this paper discusses how to calculate the paleogeological time under the condition of knowing the average reflectance of vitrinite and paleogeothermal temperature.

Coal thermodynamic equation of Wu Chonglong

When the paleogeological time and metamorphic degree are known and the paleogeological temperature is calculated:

$$\ln(\mathrm{T}-273)=\frac{646.32}{\ln t+111.85}-\frac{0.492\mathrm{t}^{0.093}}{\mathrm{R}_0} \quad (1)$$

It can be seen that the independent variables are on the right side of the equation, while the dependent variables are on the left side of the equation. The dependent variable can be obtained by directly substituting the independent variable. When the paleogeological time and paleogeological temperature are known and the metamorphic degree is calculated:

$$R_0=\frac{0.492t^{0.093}}{\frac{646.32}{lnt+111.85}-ln(T-273)} \quad (2)$$

Where: t: the author first uses "absolute age of rock stratum" and then "effective heating time", millions of years; R0: vitrinite reflectance,%, T: paleogeothermal temperature, K. It can be seen that the independent variables are on the right side of the equation, while the dependent variables are on the left side of the equation. The dependent variable can be obtained by directly substituting the independent variable. However, when we know the paleogeological temperature T and metamorphic degree R0 and calculate the paleogeological time t, there will be no matter how the term is shifted, except that the independent variable is on the right of the equation, while the dependent variable is on the left and right of the equation at the same time. For example:

$$\ln t=646.32\left(\frac{\mathrm{R}_0}{\mathrm{R}_0\ln(\mathrm{T}-273)+0.492\mathrm{t}^{0.093}}\right)-111.85 \quad (3)$$

Equation (3) has no root formula, so it is very difficult to find the exact root, so it is particularly important to find the approximate root of the equation.

Coal forming period and vitrinite reflectance

From the research reports of six coal forming periods in China, three geological periods that can produce low rank coal (long flame coal) to high rank coal (anthracite) are selected as mutually verified paleogeological periods: ① late Paleozoic Carboniferous to early Permian: about 320-278 million years ago. The time span is 42 million years, referred to as the Carboniferous. The Carboniferous is the earliest coal resource formation period. The Carboniferous coal in China is basically distributed in the Yellow River Basin, and the coal types range from long flame coal to anthracite. ② Early and Middle Jurassic of Mesozoic: about 205-159 million years ago. The time span is 46 million years, referred to as Jurassic. Jurassic coal is mainly concentrated in the junction of Inner Mongolia, Shaanxi, Gansu and Ningxia and Northern Xinjiang. The coal types range from lignite, long flame coal to anthracite. ③ Early Cretaceous of Mesozoic Era: about 142-99 million years ago. The time span is 43 million years, referred to as Cretaceous. Cretaceous coal is distributed in eastern Inner Mongolia and Northeast China. The Cretaceous coal types in the three northeastern provinces range from long flame coal to anthracite. Because the required paleogeological time should be in a certain geological period, with a difference of one million years, and it can never be in different geological periods. For vitrinite reflectance of all bituminous coals (gas coal, fat coal, coking coal, lean coal, lean coal, weakly viscous coal and non viscous coal), refer to Li Wenhua's article "relationship between average maximum reflectance of bituminous vitrinite and coal type" [9]. The classification of coalification degree (low coal grade coal, medium coal grade coal of Grade 7 and high coal grade coal of grade 3) can refer to China's coal industry standard [10].

Calculation of paleogeological time

Use iterative algorithm to solve the problem. Iteration means constant substitution. The main steps involve selecting iteration variables, establishing iteration relations, and controlling the iteration process.

Selecting iteration variables and establishing iteration relations

The so-called iterative relationship refers to the formula (or relationship) of how to deduce the next value of a variable from the previous value. The establishment of iterative relation is the key to solve iterative problems, which can usually be completed by recursive or backward methods. In the problems that can be solved by iterative algorithm, there is at least one variable that can continuously deduce new values from old values directly or indirectly. This variable is iterative variable. Equation (3) is designed as an iterative relationship.

$$\ln t_2 = 646.32\left(\frac{R_0}{R_0 \ln(T-273)+0.492t_1^{0.093}}\right) - 111.85 \quad (4)$$

Obviously, the required paleogeological time t is an iterative variable.

Golden section method

The specific operation is to substitute the known paleogeothermal temperature T, vitrinite reflectance R0 and hypothetical t1 into equation (4) to obtain t2. Generally, the iterative process is controlled by ① setting the number of iterations or ② setting the difference between the iterative values before and after determination, so as to avoid the endless execution of the iterative process. After t2 is obtained, follow-up calculation is carried out according to the following equation:

$$dt = t_2 - t_1 \quad (5)$$

$$\Delta = 0.618 * dt \quad (6)$$

It can be seen from equation (6) that the golden section value of 0.618 is used. The Golden Section [11, 12] refers to the division of the whole into two. The ratio of the larger part to the whole part is equal to the ratio of the smaller part to the larger part, and its ratio is about 0.618. This proportion is recognized as the most aesthetic proportion, so it is called the golden section.

The relationship between the new t1 re-substituted into equation (4) and the previous t1 is:

$$newt_1 = oldt_1 + \Delta \quad (7)$$

In this paper, the difference method of determining the iterative values before and after is used to control the iterative process, that is

$$|dt| \leq 1.0 \quad (8)$$

Calculation examples

It is known that for coal samples from Carboniferous, paleogeothermal temperature T = 373k and vitrinite reflectance R0 = 0.95. The iterative results are shown in Table 1, and figure 1 is the trend chart of 10 iterative values.

Table 1 Iterative results of Carboniferous coal samples with paleogeothermal temperature T = 373k and vitrinite reflectance R0 = 0.95

t_1	t_2	dt	Δ	$newt_1$
310.0	371.3	61.3	37.9	347.9
347.9	303.0	-44.9	-27.7	320.1
320.1	351.0	30.9	19.1	339.2
339.2	317.0	-22.2	-13.7	325.5
325.5	341.0	15.5	9.6	335.1
335.1	323.0	-12.1	-7.5	327.6
327.6	337.0	9.4	5.8	333.4
333.4	326.0	-7.4	-4.6	328.8
328.8	334.6	5.8	3.6	332.4
331.0	330.7	-0.3		

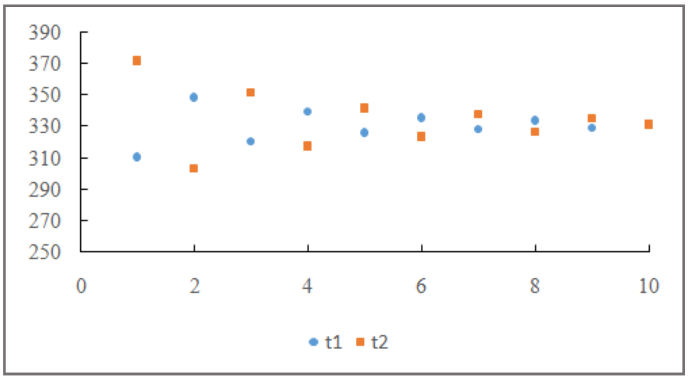

Figure 1 Trend chart of 10 iterations with paleogeothermal temperature T = 373k and vitrinite reflectance R0 = 0.95

Through 10 iterations, the paleogeological time is 331 million years. But this result goes beyond the Carboniferous period. This indicates that the given paleogeothermal temperature is low.

It is known that for coal samples from Carboniferous, paleogeothermal temperature T = 433K and vitrinite reflectance R0 = 1.7. The iterative results are shown in Table 2 and Figure 2 is the iterative trend chart.

Table 2 Iterative results of Carboniferous coal samples with paleogeothermal temperature T = 433K and vitrinite

reflectance R0 = 1.7

t_1	t_2	dt	Δ	newt_1
310.0	67.0	-243.0	-150.2	159.8
159.8	126.0	-33.8	-20.9	138.9
138.9	142.0	3.1	1.9	140.8
140.8	140.8	0.0	0.0	140.8
140.8				

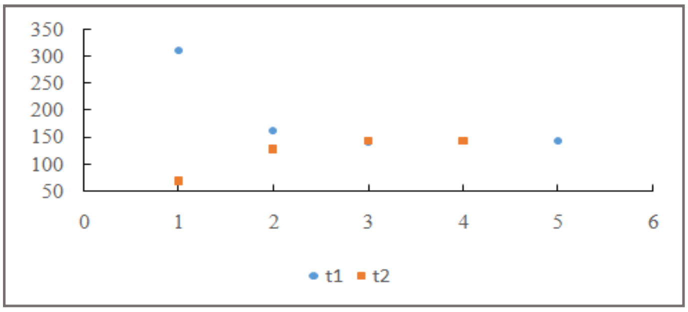

Figure 2 Trend chart of iteration with Carboniferous coal samples with paleogeothermal temperature T=433K and vitrinite reflectance R0 = 1.7

Through five iterations, the paleogeological time is 141 million years. But this result has not reached the Carboniferous geological period. This indicates that the given paleogeothermal temperature is on the high side. It is known that for coal samples from Jurassic, paleogeothermal temperature T = 414k and vitrinite reflectance R0 = 1.4. The iterative results are shown in Table 3 and the iterative trend diagram is shown in Figure 3.

Table 3 Iterative results of Jurassic coal samples with paleogeothermal temperature T = 414k and vitrinite

reflectance R0 = 1.4

t_1	t_2	dt	Δ	newt_1
310.0	104.0	-206.0	-127.3	182.7
182.7	191.5	8.8	5.4	188.1
188.1	185.3	-2.8	-1.8	186.4
186.4	187.2	0.8	0.5	186.9
186.9	186.6	-0.3	-0.2	186.7
186.7				

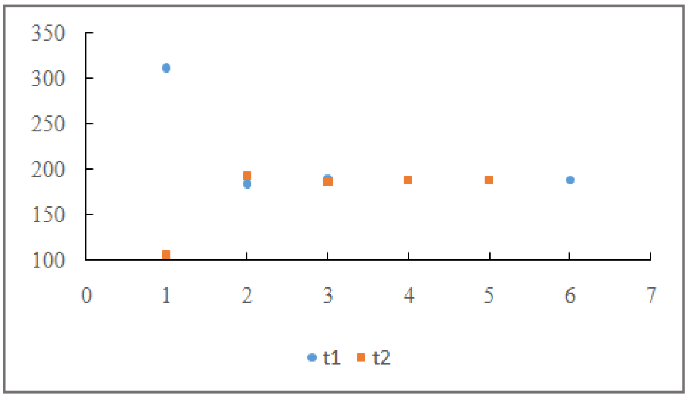

Figure 3 Trend chart of iteration with paleogeothermal temperature T = 414k and vitrinite reflectance R0 = 1.4

Through six iterations, the paleogeological time is 187 million years. But this result is in the Jurassic period. It is known that for coal samples from Cretaceous, paleogeothermal temperature T = 440k and vitrinite reflectance R0 = 1.84. The iterative results are shown in Table 4 and the iterative trend diagram is shown in Figure 4.

Table 4 Iterative results of Cretaceous coal samples with paleogeothermal temperature T = 440k and vitrinite

reflectance R0 = 1.84

t_1	t_2	dt	Δ	newt_1
187.0	94.0	-93.0	-57.5	129.5
129.5	127.7	-1.8	-1.1	128.4
128.4	128.6	0.0082		

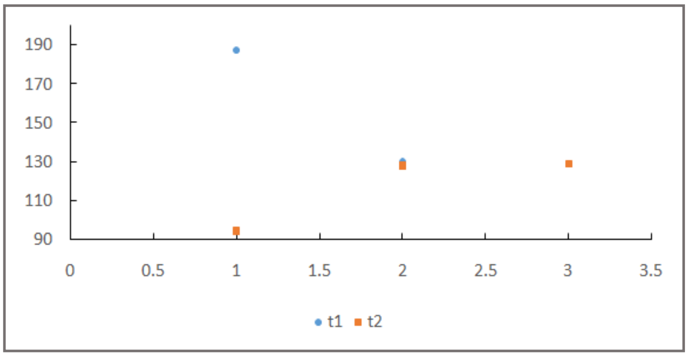

Figure 4 Trend chart of iteration with paleogeothermal temperature T = 440k and vitrinite reflectance R0 = 1.84

Through three iterations, the paleogeological time is 129 million years. But this result is in the Cretaceous period. It is known that for coal samples from Cretaceous, paleogeothermal temperature T = 353K and vitrinite reflectance R0 = 0.52. The iterative results are shown in Table 5 and figure 5 is the iterative trend chart.

Table 5 Iterative results of Cretaceous coal samples with paleogeothermal temperature T = 353K and vitrinite reflectance R0 = 0.52

t_1	t_2	dt	Δ	newt_1
128.5	0.0	-128.5	-79.4	49.1
49.1	2.0	-47.1	-29.1	20.0
20.0	18.3	-1.7	-1.0	18.9
18.9	20.9	2.0	1.2	20.2
19.5	19.4	-0.1		

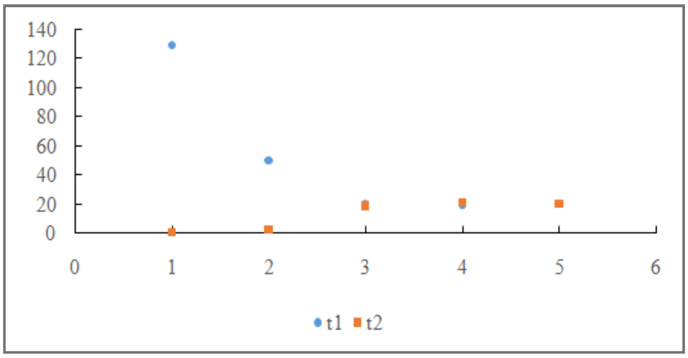

Figure 5 Trend chart of iteration with paleogeothermal temperature T = 353K and vitrinite reflectance R0 = 0.52

Through 5 iterations, the paleogeological time is 20 million years. This geological result is not yet Cretaceous. This indicates that the given paleogeothermal temperature is on the high side.

At the same time, it can be solved by computer programming. On the premise of knowing the paleogeothermal temperature and vitrinite reflectance, iterative calculation can be carried out to solve the paleogeological time in the coal thermodynamic equation.

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