

Study on Thermal History Simulation Method of Sedimentary Basin

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Abstract

The study of thermal history of sedimentary basins is an important part of basin dynamics and hydrocarbon accumulation analysis, which is of great significance for revealing the maturation and evolution of source rocks, hydrocarbon generation and expulsion processes and hydrocarbon accumulation rules. In this paper, two basic methods of basin thermal history restoration are systematically sorted out: tectonic thermal evolution method and paleotemperature scale method. The tectonic thermal evolution method is based on the dynamic model of the lithosphere scale. By simulating the tectonic subsidence and thermal effects of different types of basins such as extension, foreland, craton and strike-slip pull-apart, the basin heat flow history is obtained by forward modeling. The paleo-thermometer method uses the paleo-geothermal information recorded by the paleo-thermometer such as vitrinite reflectance, asphalt reflectance, fission track and (U-Th)/He in the sedimentary strata of the basin to invert the thermal history of the basin. The combination of the two methods can give full play to the advantages of forward modeling and inversion, and make up for the shortcomings of a single method. In addition, this paper also discusses the temperature application range of different paleotemperature scales, the progress of dynamic models and their application examples in the analysis of oil and gas basins. The research shows that the tectonic thermal evolution method is suitable for revealing the origin of the basin and the evolution process of the lithosphere, while the paleo-thermometer method, especially the low-temperature thermochronology method, can accurately describe the thermal history path of the basin. The combined use of the two methods is the development trend of the current basin thermal history research.

Keywords

Sedimentary Basin; Thermal History Simulation; Structural Thermal Evolution Method.

1. Introduction

The thermal history of the basin is an important part of the study of basin dynamics, and it is also one of the key factors in the maturation of organic matter in the sedimentary rocks of the oil and gas basin and its transformation into hydrocarbon. The organic matter needs to reach a certain temperature condition to generate oil and gas. Therefore, the maturity of organic matter is mainly controlled by temperature. At the same time, the oil and gas accumulation in the basin is closely related to temperature. The thermal history of the basin controls a series of important processes such as oil and gas discharge, migration, accumulation and preservation.

The study of thermal history of sedimentary basins is a crucial part of basin analysis. The main research includes the genetic mechanism, thermal system, thermal structure, thermal history recovery simulation and tectonic thermal events of different basins. As an important means of basin analysis, the study of thermal history of sedimentary basins can provide important information such as uplift and denudation of basins and orogenic belts, tectonic thermal

events[1]. At the same time, the thermal history of basins also controls the generation and accumulation evolution of oil, natural gas, coal and various energy minerals. A series of processes such as the generation, discharge, migration, accumulation and preservation of oil and gas are controlled by the thermal evolution history of the basin. By restoring the thermal history of the sedimentary basin, the maturity process of the source rock, the history of hydrocarbon generation and expulsion, and the location and migration process of the ' source kitchen ' in the geological history period can be revealed[2]. Therefore, the study of basin thermal history is of great significance in the field of oil and gas accumulation research and oil and gas exploration. Nowadays, the study of thermal history of sedimentary basins has become one of the frontier and difficult problems in the fields of basin dynamics and petroleum geology. The study of thermal history of basins can be carried out on two scales, namely lithosphere scale and basin scale. On the lithospheric scale, the appropriate mathematical model is selected according to the basins with different genetic mechanisms, and the model parameters are continuously adjusted. The heat flow history of the basin is obtained by fitting the actual tectonic subsidence of the basin, and then the thermal history in the basin is reconstructed by combining the geological data such as the burial history of the basin. This method is also called ' tectonic thermal evolution method '. At the basin scale, the thermal history of the basin and the heat flow history of the basin are usually inverted by using the paleotemperatures recorded by paleothermometers or paleogeothermometers such as organic matter, minerals and fluids in the sedimentary strata of the basin. This method is called ' paleothermometer method '. These two are two basic methods for the study of basin thermal history. The combination of the two is a forward and inversion method to obtain the thermal history of the basin based on the known thermal state of the basin and a certain tectonic evolution model. This method can not only verify the selected basin model and provide information such as basin genesis, but also reveal the parameters such as lithospheric extension and thickness change during the tectonic evolution of the basin. It not only utilizes the advantages of the tectonic thermal evolution method and the paleo-thermometer method, but also overcomes the shortcomings caused by the defects of the geodynamic model and the paleo-thermometer model [3].

2. Structural Thermal Evolution Method

2.1. Thermal Evolution Simulation of Basin

The tectonic thermal evolution method of basin is also called the geodynamic simulation method of basin evolution. The basic principle of the tectonic thermal evolution method is to obtain the temporal and spatial evolution history of the lithosphere in terms of temperature and heat flow by simulating various structural changes and corresponding thermal effects such as extensional thinning, flexural deformation, and isostatic adjustment during the formation of the basin. The tectonic thermal evolution method determines the appropriate mathematical model according to the corresponding geological parameters for various genetic types of sedimentary basins. Under the known or assumed initial conditions and boundary conditions, the parameters of the model are continuously adjusted to make the simulation results fit the actual observed basin tectonic subsidence history, so as to determine the basement heat flow of the basin, and then restore the thermal history of the sedimentary basin in combination with the sedimentary burial history of the basin[5].

Beaumont and Tankard[6] simplified the basin structure into five types, namely extensional, transtensional, transpressional, foreland and intracratonic basins. The tectonic thermal evolution method divides the basin into the following four main types according to the dynamic mechanism of basin formation:

(1) Extensional basins related to rifting;

- (2) Foreland flexural basins related to lithosphere shortening and flexure in the orogenic foreland area;
- (3) Craton basins related to non-orogenic granite intrusion or metamorphism;
- (4) Strike-slip pull-apart basin related to strike-slip or detachment.

2.2. Extensional Basin

The extensional basin is a kind of rift basin related to the extension and thinning of the crust and lithosphere under the action of tension. It is usually composed of a series of basin evolution sequences from intracontinental rift to passive continental margin. Its basic styles are rift basin, depression, depression trough, passive continental margin and so on[7]. The tectonic thermal effect of the extensional basin mainly includes the extension and thinning of the lithosphere, mantle emplacement and isostatic adjustment. In 1978, McKenzie[8] proposed the instantaneous uniform extension model after studying the quantitative conclusion of passive rift, which is also an earlier and widely used basin dynamics model. The model proposes mathematical expressions for calculating initial subsidence, thermal subsidence, and vertical heat transfer on the surface, which lays a theoretical foundation for quantitative models and simulation studies of extensional basins. In addition, in view of the development of basaltic dykes in many rift basins, Royden and Keen[9] proposed a dyke intrusion model in 1980 and introduced a new parameter to characterize the ratio of the crust to the replacement of asthenosphere and mantle materials. In addition, many extensional basins in the world have undergone multi-stage non-uniform tension during the evolution process. The results of multi-stage tension make the later evolution history of the basin affected by the unstable temperature field in the early stage. The thermal history and current thermal state of the basin are formed under the combined action of multi-stage tension. At present, in order to study the tectonic thermal evolution history of multi-stage extensional basins, different scholars have established different multi-stage extensional dynamic models of rift basins for important parameters of lithospheric extensional evolution such as tensile coefficient and strain rate[10]

2.3. Foreland Flexural Basin

Foreland flexural basins are mainly formed in and near the convergence of plates. They are basin types formed by compression and bending of the lithosphere due to external forces. They mainly include arc-forward continental basins and back-arc foreland basins, which are related to collision orogeny. With the rapid uplift of the orogenic belt, it is caused by the shortening of the lithosphere in the foreland area of the orogenic belt. The main controlling factors of its formation are the tectonic load of the thrust belt, the sediment load of the basin and the horizontal extrusion pressure in the crust formed during the orogenic process[11]. In the foreland flexural basin, the change of heat flow at the bottom of the basin is small, and the thermal effect of fault shear nappe in the basin plays an important role.

In 1983, Karner et al.[12] proposed a thermoelastic rheological model, which can explain the relationship between deflection and thermal evolution history. In 1985, Willett et al.[13] proposed a viscoelastic rheological model, which can explain the relationship between the stiffness of the lithosphere and the loading time. Both the thermoelastic rheological model and the viscoelastic rheological model are the mathematical models of the lithosphere deflection in the foreland flexural basin. The mathematical models of the load include the unilateral critical vertebral body model and the bilateral critical vertebral body model. Compared with extensional basins, the quantitative model of foreland flexural basins is more concerned with the tectonic subsidence of the basin, and the research on the tectonic thermal effect of the basin is not enough.

2.4. Cratonic Basin

The craton is a stable block located on the crystalline Precambrian basement, Mesozoic basement, or even on the rifted or other accretive continental lithospheric material. The cratonic basins are all sedimentary areas that are deposited on top of the craton, including, in particular, those located on long-term stable, weakly deformed basements, or on top of early rifts and other types of basins, mainly within the craton. Compared with extensional basins and foreland flexural basins, craton basins have complex genetic mechanisms and evolution models, including crustal extension, thermal attenuation, intraplate stress, undercompensated mass, and craton marginal tectonic load.

Due to the complex geodynamic evolution process of the cratonic basin, its evolution process has stage characteristics. Different quantitative mathematical models of the basin can only be applied to some specific stages of the basin evolution process. The craton basin is similar to the back-arc continental rift basin in terms of crustal extension and thermal subsidence, but its lithospheric and crustal extension scale and thermal subsidence are relatively small, and the thermal subsidence shows stage characteristics, so the thermal subsidence is only applicable to some stages of basin development[14]. Craton basins are usually considered to be caused by the intrusion of granites in the post-orogenic crust or the metamorphic reaction in the deep crust. Due to the temporal and spatial changes of magmatic activity and metamorphism, the metamorphic model proposed by Middleton and Foster[15] can be applied in some stages of basin development.

2.5. Strike-slip Pull-apart Basin

The strike-slip pull-apart basin is a basin related to strike-slip faulting. According to the mechanical properties and subsidence history of strike-slip pull-apart basins, they are usually divided into two main types : one is related to thin-skinned detachment structures, there is no deep thermal disturbance, and only one cooling process is experienced, which belongs to ' cold basin ' ; the other type of scale continues to expand, resulting in the upwelling of the mantle, from the passive rift into the active rift, which belongs to the ' hot basin ' .

In the selection of quantitative mathematical model of basin, the first type can be thin-skinned structure model[16], and the second type can be extensional basin model. Because the rapid subsidence in the early stage of strike-slip pull-apart basin development is caused by crustal extension and lateral heat transfer, only the initial subsidence caused by shallow crustal extension, and the continuous thermal subsidence in the late stage is limited, the extension model needs to be modified in application[17].

3. Ancient Temperature Scale Method

The paleothermometer method is another method to study the thermal history of sedimentary basins. Different from the tectonic thermal evolution method, the paleothermometer method uses the paleothermometer (also known as the ' paleogeothermometer ') preserved in the sedimentary basin to invert the thermal history of the sedimentary basin, which can be divided into direct inversion and indirect inversion. The direct inversion is to divide the thermal history path of the paleothermometer sample into multiple time periods. Different models are applied in each time period, and the theoretical value of the model is calculated by forward modeling. The difference between the theoretical value and the measured value is iterated repeatedly, which is only applicable to the thermal history path of linear warming or linear cooling. The basic principle of indirect inversion is an iterative process based on the reconstruction of burial history and the simulation of physical processes in the basin, with the paleo-thermometer dynamic model as the core. Indirect inversion is to determine the thermal history path of the formation indirectly according to the burial history of the basin by taking the attenuation of

heat flow change p at the bottom of the basin and the erosion amount H of the formation as the selection parameters[18].

The organic matter or mineral in the sedimentary basin undergoes a series of changes in physical and chemical properties by heating, thus recording the paleogeothermal information, so it is called the paleotemperature scale. Each paleothermometer has a specific temperature range : some paleothermometers are the highest paleothermometers, which can only record the highest paleotemperature they have experienced, such as R_o ; some can record the thermal history of the sample, such as fission track.[19] At present, there are mainly two types of paleothermometers, organic paleothermometers and low-temperature thermochronology paleothermometers, which are relatively mature and widely used. The combined use of them has become an effective way and trend to study the thermal history of sedimentary basins.

3.1. Organic Matter Paleotemperature Scale

Organic matter paleothermometer is the most common type of paleothermometer. Its principle is to use the relationship between the maturity of organic matter contained in sedimentary strata and formation temperature to restore or reconstruct the formation temperature history of sedimentary basins. The chemical composition, structure and physical properties of the organic matter deposited in the sedimentary process of the basin change during the thermal degradation process, and each maturity index is related to specific chemical kinetics and temperature. The organic matter paleothermometer includes vitrinite reflectance, asphalt reflectance, vitrinite reflectance, fluorescence of organic matter, sporopollen color and thermal variability index[20].

3.1.1. Vitrinite Reflectivity

Vitrinite reflectance is the most reliable indicator of organic matter maturity, and it is also the most commonly used organic matter paleothermometer method in the study of thermal history and oil and gas geology of sedimentary basins. With the passage of time, the organic matter in the sedimentary strata is continuously matured by the effect of ground temperature for a long time, and the degree of condensation of aromatic rings in the molecular structure of vitrinite increases, forming more dense structural units, thus increasing the reflectivity of vitrinite[21]. In order to invert the thermal history of sedimentary basins by using vitrinite reflectance, the sedimentary burial history of the basin should be reconstructed first. The detailed sedimentary burial history is the basis for studying the paleogeotemperature of the basin. Secondly, assuming a paleogeothermal gradient or heat flow model, combined with the burial history, the paleogeothermal experienced by the stratum where the sample is located is calculated. Again, the maturity of the layer where the sample is located is calculated from the ancient ground temperature ; then, the measured maturity and the calculated maturity are compared. By repeatedly modifying the assumed paleogeothermal gradient model and repeatedly calculating the maturity, the calculated maturity and the measured maturity are fitted. Finally, the selected paleogeothermal gradient model and the thermal history calculated based on it can represent the paleogeothermal gradient of the basin and the thermal history experienced by the stratum where the sample is located[22].

In the process of simulating thermal erosion of sedimentary basins by vitrinite reflectance, it is necessary to adopt an appropriate chemical kinetic model of vitrinite reflectance. At present, the most widely used model in China is the Easy % R_o model proposed by Sweeney and Burnham in 1990, which is the most accurate method for predicting R_o .[23] The Easy % R_o model has a wide range of applicability to the recovery of paleogeothermal in different evolutionary history processes and different types of basins. It is more accurate in the application of medium maturity to high maturity. However, when the maturity is low ($R_o < 0.9$ %), the Easy % R_o model may overestimate R_o , while the Middleton et al. ' s model may be more accurate.

3.1.2. Asphalt Reflectance and Vitrinite Reflectance

In the study of Lower Paleozoic strata and marine strata, due to the lack of maceral-vitrinite of higher plants, the mature vitrinite reflectance model cannot be applied. Therefore, asphalt reflectance and vitrinite reflectance are used instead of vitrinite reflectance. The commonly used method is to convert asphalt reflectance and vitrinite reflectance into vitrinite reflectance, and the converted values are collectively referred to as equivalent vitrinite reflectance.

3.2. Low Temperature Thermochronology Paleotemperature Scale

Thermochronology is a theory and research method that applies the theory of thermal diffusion to link the interpretation of age results with the thermal evolution history of geological bodies. It uses mineral closure temperature to interpret isotope geological age data and quantitatively gives the temperature-time trajectory of geological processes. Theoretically, thermochronology can provide thermal history information in the range of 65 ~ 650 °C. The commonly used methods include U-Pb method, $^{40}\text{Ar} / ^{39}\text{Ar}$ method, fission track method, (U-Th) / He method and so on (Fig.1). However, in the process of studying the tectonic evolution of sedimentary basins and the uplift of mountains, due to the low temperature, apatite and zircon fission track and (U-Th) / He and other low temperature thermochronological methods are usually used. The He closure temperature of apatite is low, about 75 °C [24], and the fission track closure temperature is about 110 ~ 125 °C. The He closure temperature of zircon is about 170 ~ 190 °C, and the fission track closure temperature is about 210 ~ 240 °C. The He closure temperature of titanite is about 191 ~ 218 °C, and the fission track closure temperature is about 265 ~ 310 °C (titanite is less used in the study of thermal history of sedimentary basins).

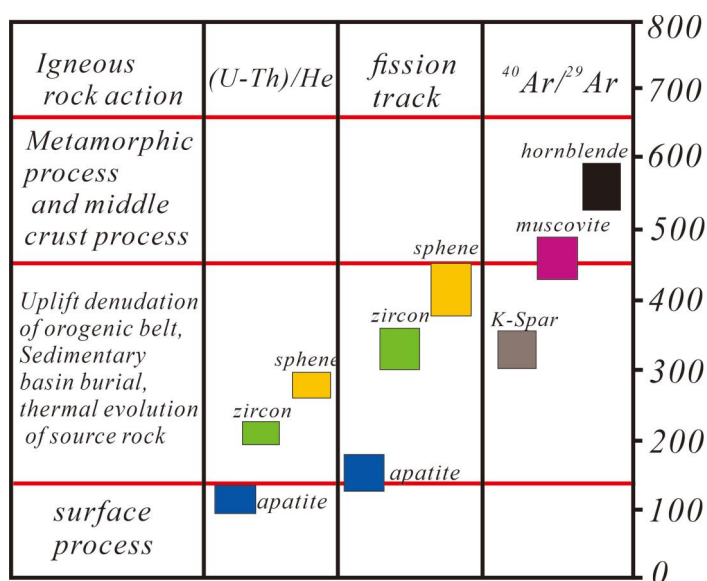


Fig 1. The applicable temperature range of different low temperature thermochronology methods

In recent years, with the improvement of quantitative models and the rapid development of testing instruments, low-temperature thermochronology has been widely used in geological body dating, basin thermal history restoration, topography evolution and sediment source research, hydrothermal fluid migration research and other aspects, and has achieved a lot of results. In particular, the temperature range of partial annealing zone of apatite fission track is 70 ~ 125 °C, which is roughly consistent with the hydrocarbon generation window on the time scale of geological history, so it can be used to study the beginning and duration of hydrocarbon generation, expulsion and migration in oil and gas basins[25].

3.2.1. Fission Track

The fission track method is a low-temperature thermochronological paleothermometer method developed rapidly in the field of basin thermal history research in the past 30 years. This method is based on the fact that the track generated by the fission of ²³⁸U contained in the mineral is affected by temperature during the geological time, and the annealing behavior occurs (that is, the fission track shows the characteristics of track length reduction and density reduction with the increase of temperature). Based on the number of tracks generated by spontaneous fission of U and Th radioactive isotopes in minerals and the rate of spontaneous fission. In sedimentary basins, the track length, track density, track age and other parameters of mineral fission track will show different characteristics due to the influence of time and temperature due to the different sedimentary strata. Naeser et al.[26] believed that there is a different relationship between fission track age and depth or temperature when the formation is at the maximum burial depth and cooled by uplift and denudation. When the basin is continuously deposited and the current temperature of the strata is the highest geothermal temperature in the geological history, the fission track age of the minerals will appear in three zones on the depth or temperature map, from shallow to deep : unannealed zone, the strata have not been annealed, and the age reflects the age of the source, greater than or equal to the age of the strata ; in the partial annealing zone, the strata have been annealed, and the age gradually decreases, which is less than the age of the strata. Complete annealing zone, age is equal to 0, the formation reached complete annealing. If the formation reaches the maximum ground temperature, due to the influence of uplift and denudation or the decrease of ground temperature gradient, the formation temperature decreases and the minerals are cooled. The fission track age of the minerals will appear with the depth or temperature map. There are five zones, from shallow to deep : unannealed zone, partially annealed zone, cooled zone, partially annealed zone, and completely annealed zone. The minerals in the cooling zone produce new fission tracks after cooling. According to the age of these tracks, the slope of the age-depth curve and the thickness of the formation, the time and rate of the cooling event and the information of the formation uplift and erosion can be determined.

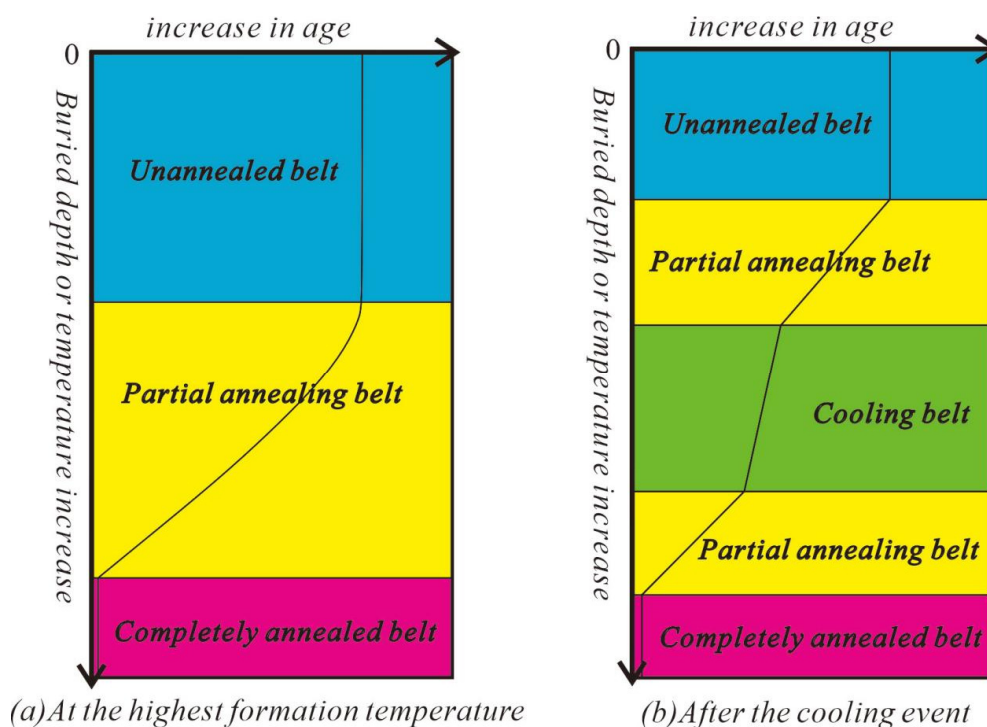


Fig 2. Division of apatite fission track annealing zone

Using fission track to study the thermal history of sedimentary basins includes two methods : forward modeling and inversion. The so-called forward modeling method is to simulate the length distribution evolution of the fission track and the final length distribution along the known thermal history path. The simulated track length distribution is compared with the measured fission track length distribution to obtain the actual thermal history evolution path of the sedimentary basin. The inversion method is to infer the thermal history path of the sedimentary basin based on the measured parameters such as the length distribution of the fission track and the age of the fission track. The source parameters and the current geothermal field parameters are used to determine the starting and ending parameters of the simulation, and the random approximation method is used to compare the thermal history of the sedimentary basin. In the process of using fission track to study the thermal history of sedimentary basins, the emphasis is on the combination of track length and track age. Simply relying on track length or track age to simulate often causes the deviation of the results. The apparent age of fission track alone has no direct geological significance, and it is necessary to simulate the thermal history by combining the length distribution of fission track and the annealing kinetic parameters. Ren[27] used apatite fission track to analyze the thermal history experienced by the Ordos Basin, and combined it with the inclusion and vitrinite reflectance data. The analysis results revealed the difference in denudation amount of different tectonic units in the Ordos Basin. In the Cretaceous period, it experienced a higher geothermal gradient and terrestrial heat flow than today, and a cooling event occurred before 20 ~ 23Ma. Tian Yuntao et al.[28] used apatite fission track results to constrain the erosion-evolution history of the Micangshan-Hannan Cangqiong-Branch since the Cretaceous. The age distribution of fission track in this area gradually became new from the south of the Hannan dome to the north of the Sichuan Basin, and experienced two periods of rapid erosion.

3.2.2. The (U-Th)/He

The (U-Th) / He dating method is the same as other radioactive dating methods, which mainly uses He produced by radioactive decay of U and Th for mineral dating. This method was first proposed by Strutt 100 years ago, but has not been widely studied and applied. In 1987, Zeitler et al.[29] proposed that the He age is the cooling age at lower temperatures, and believed that the (U-Th) / He dating method may have great potential in studying the low temperature cooling age of rocks. With the popularity of laser heating technology and laboratory automation, the (U-Th) / He dating method has been widely used in various research fields.

Minerals such as apatite are the main minerals used in the (U-Th) / He dating method because they contain more radioactive elements such as U and Th. The ^4He (U-Th) / He dating system is a closed system in which the radioactive elements ^{238}U , ^{235}U and ^{232}Th are released while the α -particle decays to produce ^{206}Pb , ^{207}Pb and ^{208}Pb . The prerequisite for using this dating method is that all the He in the mineral crystal comes from the decay of radioactive isotopes such as U and Th, and there is neither He inheritance nor He loss. Therefore, any factor that destroys the (U-Th) / He dating closed system and causes the change of He content in mineral crystals will affect the accuracy of the dating method. The reasons for the destruction of the (U-Th) / He closed dating system are divided into external and internal factors : external factors include tectonism, magmatism, thermal effects, etc. ; the internal causes include the migration distance of α particles, the diffusion behavior of He, particle size and mineral inclusions.

4. Discussion and Conclusion

The study of thermal history of sedimentary basins is a frontier and hot issue at present, and the recovery of thermal history mainly includes two aspects : one is to use the tectonic thermal evolution method to select the appropriate mathematical model for basin simulation on the

lithospheric scale ; secondly, on the basin scale, the thermal history of the basin is inverted and reconstructed by using a variety of paleothermometer methods. The method of thermal history recovery is from simple to complex, and the tectonic thermal evolution method and the paleotemperature scale method have experienced a development process from qualitative to semi-quantitative and then to quantitative[30].

Due to the close relationship between basin subsidence and basin thermal effect, the geodynamic background and tectonic thermal evolution history of different types of sedimentary basins in different tectonic units are different. It is a common method to restore the tectonic thermal evolution history of sedimentary basins by using the geodynamic model of basin tectonic evolution[31]. However, the tectonic evolution process of the basin is extremely complex, and the existing quantitative mathematical model of the basin is too simplified compared with the geological process, which can only reflect the main tectonic thermal process in the geological history of the basin. In addition, due to the great uncertainty in the selection of basin model parameters, although the simulation results of basin tectonic thermal evolution given by the mathematical model of the basin are quantitative, they can only be regarded as semi-quantitative to a certain extent [32].

Compared with the tectonic thermal evolution method, the paleothermometer method can fit the simulation results with the paleogeothermal information recorded in organic matter or minerals, so as to obtain a more accurate basin thermal history. Vitrinite emissivity is the most reliable indicator of organic matter maturity. It is widely used in research fields including basin thermal history recovery and many fields in the petroleum industry. However, the acquisition of vitrinite requires certain conditions. Therefore, after a lot of research, scholars have established the calculation formula of equivalent vitrinite reflectance associated with organic matter paleothermometer such as asphalt emissivity and vitrinite reflectance, which is used to calculate the thermal history of strata lacking vitrinite reflectance, such as marine carbonate strata. Low-temperature thermochronology has become an important paleothermometer method in the study of basin thermal history due to the continuous improvement of theoretical basis and the great improvement of experimental instrument accuracy in recent years. Its advantage is that it can record the thermal history process experienced by paleothermometer samples, which is impossible for the highest paleothermometer. Since the fission track of different minerals and the closure temperature of (U-Th) / He are different, the thermal history paths of different temperature ranges in the basin can be studied by combining the fission track of various minerals with the (U-Th) / He dating method [33]. With the improvement of the existing paleothermometer method, new paleothermometer methods are constantly being explored and applied to the study of basin thermal history, such as organic matter free radical concentration, rock thermal acoustic emission and so on.

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