

Research on Methods of Thermal History Reconstruction

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Abstract

This paper centers on methods for thermal history reconstruction. By outlining the development of the basin simulation system, it points out that a complete basin simulation framework includes the sedimentation history, thermal history, organic maturation history, and basin fluid model. Different dimensions of models are required at various exploration stages, and such models have wide applications in the field of petroleum geology. The core focuses are two categories of methods for thermal history reconstruction: First category: lithospheric-scale forward thermal-geodynamic modeling (geodynamics approach). Based on heat transfer principles and basin evolution characteristics, mathematical models are used to simulate lithospheric structure and thermal effects to recover the thermal history. This approach is suitable for the exploration-early stage of basins, but it suffers from high parameter uncertainty and relatively low accuracy. Second category: basin-scale paleotemperature (geotherm) inversion modeling. By inverting the thermal history with various paleotemperature indicators, this category details the principles, applicability, and advantages and disadvantages of multiple specific methods. The abstract also proposes a new basin thermal modeling pathway that combines the two methodologies. It identifies the current mainstream approaches and the development trends of basin thermal modeling and emphasizes the need for integrated methods and consideration of multiple factors to accurately reconstruct the thermal evolution history of basins, thereby supporting descriptions of oil and gas accumulation and resource assessment.

Keywords

Thermal History Simulation; Forward Modeling; Paleotemperature (Geotherm) Inversion.

1. Introduction

Basin simulation is based on the geological mechanisms of physical chemistry. By means of computer technology, it quantitatively simulates the formation and evolution of petroliferous basins as well as the generation, migration and accumulation of hydrocarbons in both temporal and spatial dimensions, so as to reveal the inherent laws of oil and gas in basins.

As early as 1978, the Institute of Petroleum and Organic Geochemistry of Jülich Nuclear Research GmbH (Federal Republic of Germany at that time) established the world's first one-dimensional basin simulation system, thus pioneering the "basin simulation" technology. In 1984, the French Petroleum Institute developed a relatively complete two-dimensional basin simulation system, which could calculate the burial history, paleo-heat flow history, hydrocarbon maturity history and oil accumulation history. In 1987, British Petroleum Company took the lead in incorporating the theory of multiphase fluid migration into the two-dimensional model. In this model, hydrodynamic force and buoyancy are regarded as the

driving forces for multiphase fluid migration, and it is currently a well-recognized model publicly published regarding the secondary migration of oil and gas. In addition, scientists have continuously supplemented and improved the simulation theories and methods. For example, in 1984, the Department of Geology of the University of South Carolina (USA) proposed a method for determining paleo-heat flow using vitrinite reflectance; in 1981, the Exploration Department of Japan Petroleum Exploration Co., Ltd. incorporated the calculation of hydrocarbon generation amount and expulsion amount into its two-dimensional basin simulation system. Subsequently, the one-dimensional hydrocarbon expulsion model was supplemented and improved in 1987. By the 1990s, with the successive publication of Quantitative Sedimentary Basin Modeling by Angevine et al. And Quantitative Methods in Sedimentary Basin Analysis by Lerche et al., the theory of basin simulation became more comprehensive, and the simulation system software also became more practical [1-2].

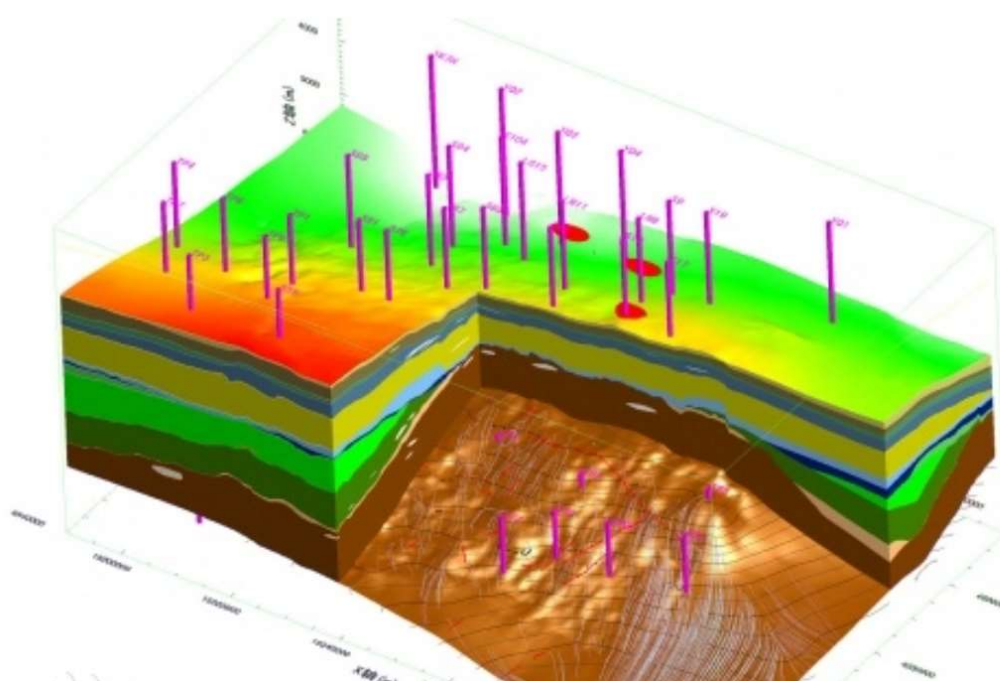


Fig. 1 Basin Simulation Model

Basin simulation research is widely applied in the field of petroleum geology. Its simulation content not only covers the research on basic geology during basin evolution, such as sedimentation, subsidence, heat flow and paleogeotemperature, but also includes studies on various aspects like the chemical kinetics of hydrocarbon generation-kerogen cracking process, hydrocarbon expulsion kinetics, and hydrocarbon resource evaluation.

2. Basin Simulation System

At present, a complete basin simulation system is organically composed of the following four models: subsidence history model, thermal history model, organic matter transformation history model, and basin fluid model. In practical application, the dimension adopted by each model shall depend on the exploration degree:

At the high exploration degree stage (i.e., with sufficient wells and seismic coverage), 3D simulation is appropriate; At the medium exploration degree stage (i.e., with limited wells and seismic coverage), 2D simulation is suitable; At the low exploration degree stage (i.e., with only a few wells), 1D simulation should be used.

Due to the numerous simplified assumptions of the above-mentioned models themselves and the uncertainty of input data: No secondary migration simulation can be conducted at the low exploration degree stage; At the medium exploration degree stage, the system plays a role in play evaluation; At the high exploration degree stage, it basically still functions in play evaluation, and only may serve the purpose of trap evaluation in local areas.

It can be seen from this that it will take a long time of efforts for basin simulation technology to truly become a quantitative tool for petroleum systems or hydrocarbon accumulation dynamics (source rock-trap).

2.1. Subsidence History Simulation

Subsidence history analysis is a conventional technique in basin analysis. By quantitatively reconstructing the amount of historical subsidence to reproduce geological history, it enables the study of basin tectonic driving mechanisms, formation and evolution, as well as the thermal evolution and hydrocarbon generation window of petroliferous basins. Additionally, it can restore stratal characteristics and changes in rates, providing a spatiotemporal framework for other simulations, and has been widely applied in recent years. Through the vertical movement pattern of stratigraphic horizons, the subsidence and uplift of a specific point in the basin can be tracked. This process requires data such as stratigraphic thickness, lithology, paleowater depth, and age constraints, which can be used to restore the original thickness of strata and calculate subsidence rates-making it a prerequisite for other basin simulations.

First, a sedimentary accumulation graph is plotted based on the current thickness and age of the strata. Then, after undergoing decompaction correction and paleowater depth correction, a total subsidence curve that incorporates multiple influencing factors is obtained. Quantitative simulation is divided into inversion (backstripping) and forward modeling methods. The backstripping method can eliminate the influence of sedimentary load, resulting in a subsidence curve that reflects tectonic factors. In the central-southern part of the Ordos Basin, researchers calculated the amount of subsidence through single-well backstripping inversion based on drilling data. They analyzed the subsidence rate and the law of center migration by combining well locations and curve characteristics, and discussed the subsidence mechanism in the context of regional tectonics.

2.2. Thermal History Simulation

The purpose of thermal history simulation is to simulate the paleogeotemperature history and paleogeothermal history of a basin. Paleogeotemperature plays a crucial role in the diagenesis and mineralization of sediments-various petrochemical changes and mineral transformations all take the ambient temperature as a key condition. For instance, in the process of hydrocarbon generation and transformation from organic matter, geotemperature is a decisive factor.

The research methods for basin thermal history mainly rely on test data to infer paleogeotemperature. Examples include using indicators such as organic matter maturity indices, conodont color alteration index (CAI), fission track dating, and fluid inclusions to calculate paleogeotemperature. This section focuses on introducing the methods of basin thermal history simulation based on thermodynamics principles. Currently, there are two most common methods: one is the geothermodynamic method, and the other is the thermal indicator inversion method.

2.3. Organic Matter Transformation History Simulation

The simulation of organic matter transformation history, i.e., hydrocarbon generation history, includes two parts: organic matter maturity history and hydrocarbon generation history. The simulation of organic matter transformation history provides a quantitative basis for the prospect evaluation of basin hydrocarbon resources, and it serves as the foundation for simulating hydrocarbon expulsion history and migration-accumulation history.

The four stages of organic matter evolution represent the entire process from the beginning of sedimentation to the end of evolution. In some basins, the evolution of organic matter may stop at a certain stage due to changes in geological factors. From an evolutionary perspective, with the increase of geotemperature and burial depth, the evolutionary stage continues to advance. Organic matter in some ancient strata may have mostly transformed into natural gas and bitumen. Therefore, in basins where organic matter is in the high-maturity or over-maturity stage, the possibility of finding oil is relatively low, while natural gas resources are highly likely to be discovered.

Due to the differences in geological environments and evolutionary histories of different sedimentary basins, the processes of hydrocarbon generation and coalification may vary significantly. These processes themselves are extremely complex, and their variability further increases the difficulty of studying them. Since World War II, numerous super-large oil fields, gas fields, and coal fields have been successively discovered, which has greatly promoted social development.

2.4. Basin Fluid Simulation

Basin fluid flow is the result of the combined effects of basin dynamic setting, tectonics, sedimentary filling, and thermal history. The purpose of basin fluid simulation is to reconstruct the laws of fluid activity during basin evolution, including the temporal changes of parameters such as sediment physical properties, temperature field, pressure field, fluid flow velocity, flow rate, and water-rock interaction rate during basin evolution. Furthermore, it can provide a basis for the migration and accumulation of oil and gas, as well as the migration and accumulation of ore-forming fluids in the basin. Therefore, basin fluid simulation serves as the foundation for simulating the migration and accumulation of ore-forming fluids or oil and gas, and it is also an indispensable link in the evaluation of geological resources within the basin.

There are two methods for basin fluid simulation: one is the analytical method, and the other is the numerical method. The former directly solves the mathematical model using mathematical methods such as integration or integral transformation, and the solution obtained is the exact solution of the mathematical model; the latter solves the mathematical model using a discretization method, and the solution, which is a set of numerical values, is the approximate solution of the mathematical model. In basin fluid simulation, since fluid activity occurs in a heterogeneous and complex stratigraphic system, the analytical method requires making various assumptions about the research object-for example, assuming that the strata are homogeneous and the boundaries have simple geometric shapes. The results of such analytical solutions can clearly and concisely reveal the general laws of basin fluid movement. However, sedimentary basins are extremely complex, and the simple assumptions made by the analytical method cannot fully reflect the actual conditions of the strata, such as anisotropy, special boundary conditions, and irregular changes during basin evolution. The use of the numerical method to solve the mathematical model just makes up for the shortcomings of the analytical method. It usually discretizes the research range (i.e., conducts grid division), and then jointly solves the grid equations of the simulation area to obtain a set of numerical solutions. Therefore, the numerical method has become the most important method in the quantitative simulation of basin fluids.

3. Thermal History Reconstruction

The reconstruction of thermal history in petroliferous basins is not only indispensable for describing hydrocarbon accumulation processes-such as determining the hydrocarbon generation stages of source rocks, organic matter maturity history, primary migration volume, play evaluation, and even trap evaluation-but also serves as a crucial aspect in studying the basin's tectono-thermal evolution process.

At present, thermal history reconstruction methods at home and abroad can be categorized into two major types: The forward modeling method for tectono-thermal evolution on the lithospheric scale, also known as the geodynamic method. This method reconstructs the basin's thermal evolution history based on geothermal transfer principles and the basin's evolutionary characteristics. The paleothermometer inversion modeling method on the basin scale. This method reconstructs the basin's thermal evolution history using various basin-scale paleothermometers, mainly including four approaches: fitting calculation of basin paleogeotemperature (stochastic inversion), basin thermal evolution history (paleogeothermal gradient method), thermal flow history at the basin bottom (paleo-heat flow history), and apatite fission track dating.

The combination of tectono-thermal evolution forward modeling and paleothermometer inversion modeling provides a new approach for studying basin tectonic evolution through the dynamic thermal regime of sedimentary basins-namely sedimentary basin thermal simulation-which integrates the research of shallow and deep tectono-thermal processes.

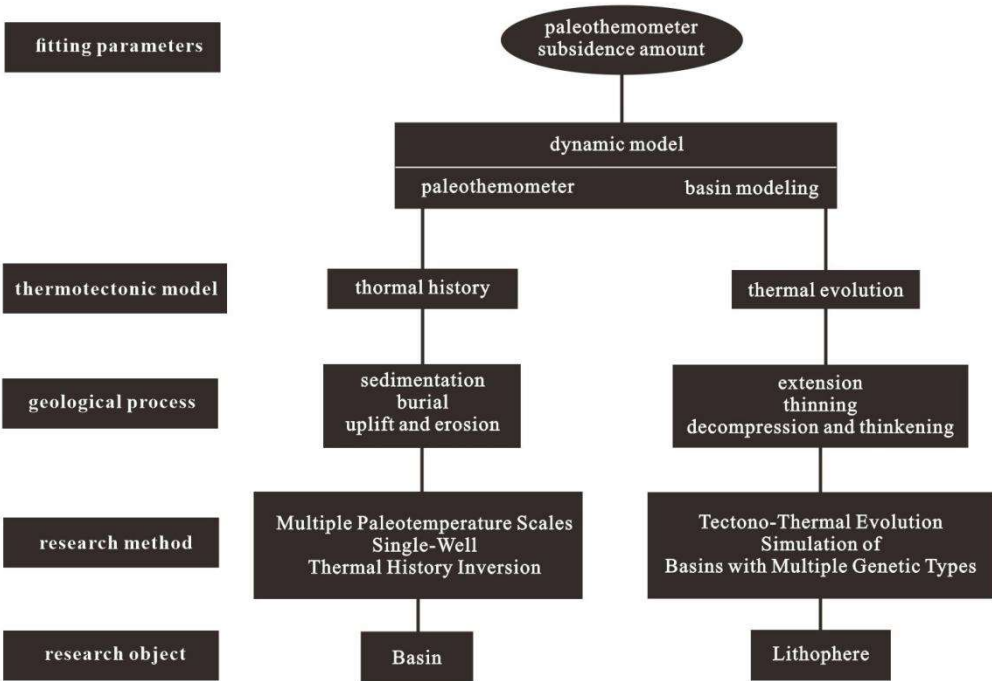


Fig. 2 Basic Framework and Principles of the Basin Thermal History Reconstruction System

3.1. Forward Modeling Method for Tectono-Thermal Evolution

The forward modeling method for tectono-thermal evolution (geodynamic method) realizes thermal history reconstruction on the lithospheric scale by simulating the tectono-thermal evolution of basins with different genetic types and their underlying lithosphere with the help of mathematical models. This method is suitable for basins in the early exploration stage that lack deep geological data.

The basic principle of forward modeling for tectono-thermal evolution is to obtain the thermal evolution of the lithosphere (temporal and spatial changes in temperature and heat flow) by simulating the lithospheric tectonics (extensional thinning, isostatic adjustment, flexural deformation, etc.) and corresponding thermal effects during the formation and development of the basin (quantitative basin model). For basins of different genetic types (rift basins, cratonic

basins, foreland basins, etc.), based on the corresponding basin mathematical models, under known or assumed initial and boundary conditions, the model parameters are adjusted to make the simulated calculation results fit the actually observed tectonic subsidence history of the basin, thereby determining the thermal flow history at the basin bottom. Furthermore, the thermal history of the strata in the basin is reconstructed by combining with the burial history of the basin.

The advantage of tectono-thermal evolution simulation is that it can grasp the general trend of regional geothermal flow evolution and predict the thermal history of un-drilled areas. However, due to the extreme complexity of basin evolution and structure, there is great uncertainty in determining the genetic type of the basin and selecting relevant parameters. Therefore, this method is often relatively rough, and the prediction accuracy is low when the existing quantitative basin models are applied to local areas. Consequently, the forward modeling of tectono-thermal evolution and the matching of forward and inversion models still need further improvement.

3.2. Paleothermometer Inversion Modeling Method

The paleothermometer method uses paleothermometers to invert the thermal history of strata and the heat flow at the basin bottom. The main approaches include vitrinite reflectance (Ro), vitrinite reflectance gradient, apatite fission track dating, EASY%Ro method, conodont color alteration index (CAI), authigenic mineral assemblage, fluid inclusion thermometry, oxygen isotope (^{18}O) analysis, and $^{40}\text{Ar}/^{39}\text{Ar}$ dating [3].

The basic principle of inverting and fitting basin thermal history using paleothermometers is as follows: A specific physical or chemical property of a paleothermometer-i.e., the currently measured paleothermometer value-depends on the temperature changes during its burial process. If the burial history is known, the thermal history can also be determined. Paleothermometer inversion methods can be further divided into direct inversion and indirect inversion [1].

Direct inversion: Directly infers the thermal history path of a sample from paleogeotemperature, including the stochastic inversion method and the paleogeothermal gradient method.

Indirect inversion: First inverts the basin's heat flow history and stratal denudation amount using paleothermometers, then indirectly reconstructs the stratal thermal history by restoring the basin's burial-denudation history and simulating the corresponding geothermal field. The core approach under this category is the paleo-heat flow method.

3.2.1. EASY%Ro Method

The EASY%Ro method model proposed by Sweeney J J et al. is developed based on the analysis of a large number of samples, considering the variation of vitrinite components with time and temperature. The thermal maturation process of vitrinite basically follows the first-order chemical kinetic equation and the Arrhenius equation-meaning the degree of thermal evolution has an exponential relationship with the heating temperature and a linear relationship with the heating time.

The EASY%Ro method, built on thermal simulation and theoretical calculation, respectively derives the activation energies required for a series of parallel chemical reactions during the thermal evolution of organic matter (such as dehydration, decarboxylation, demethylation, and removal of high-carbon-number alkyl groups) and determines their distribution ranges. Subsequently, a mathematical model is established in accordance with the principles of Arrhenius chemical reaction kinetics to quantitatively simulate the evolutionary process of vitrinite reflectance [4].

The EASY%Ro kinetic simulation method is suitable for simulating basin models with moderate to high thermal evolution degrees; however, it is no longer applicable to basin models with low evolution degrees. In addition, when using the EASY%Ro method to invert thermal history, there are issues such as insensitivity to the early stage of the studied time period, and in some cases, a strong dependence on the current geothermal gradient.

3.2.2. Vitrinite Reflectance Inversion

The magnitude of vitrinite reflectance (Ro) in strata at a specific depth within a basin is mainly controlled by the burial history of the strata where the vitrinite is located and the geothermal gradient. Once the burial history of the strata is determined, Ro is uniquely constrained by changes in the geothermal gradient. If only heat conduction- the most dominant heat transfer method in basins-is considered, the geothermal gradient depends solely on the basin's heat flow density and the thermal conductivity of its sediments; if the thermal conductivity of the sediments is also known, changes in the basin's heat flow density uniquely determine changes in the basin's geothermal gradient. Thus, under the premise of knowing the basin's burial history and sediment thermal conductivity, changes in the basin's heat flow density become the sole factor controlling the Ro value of strata at a specific depth. Therefore, based on a series of theoretical models such as the paleo-heat flow model, paleogeothermal model, and Ro model, the variation in the basin's terrestrial heat flow density can be derived through inversion using measured Ro data. Subsequently, the paleogeothermal history experienced by the basin can be obtained through forward modeling by combining the variation in the basin's heat flow density with the strata burial history and sediment thermal conductivity [5].

The Ro inversion process takes the basin dynamic model and its sedimentary-tectonic evolution history as external constraints, and uses measured vitrinite reflectance data (Roi) to progressively fit the undetermined parameters in the paleo-heat flow model. These parameters mainly include those related to the paleo-heat flow model, paleogeothermal model, and vitrinite reflectance model. By adjusting these undetermined parameters, the error between the theoretically calculated Ro values and the measured values is limited to an acceptable range; at this point, the values of these undetermined parameters are the optimal values. Substituting these optimal parameter values into the paleo-heat flow model, the basin's heat flow history, geothermal history, and organic matter maturity (Ro) history can be simulated through forward modeling based on the paleo-heat flow model, paleogeothermal model, and Ro model [5-6].

Vitrinite reflectance (Ro) at different depths in the same basin reflects changes in the heat flow density experienced by the basin. The basin's evolutionary history can be characterized by establishing the basin's paleo-heat flow, paleogeothermal, and vitrinite reflectance models. However, Ro exhibits non-uniqueness and irreversibility in polycyclic basins. Therefore, when using Ro for basin inversion, efforts should start with the restoration of the original basin, and reliable Ro data should be exploited to the maximum extent.

3.2.3. Apatite Fission Track

The reconstruction of basin thermal history using mineral fission tracks is one of the newly developed research fields that has advanced rapidly in the past decade. Currently, fission tracks in apatite and zircon are mainly used: the suitable temperature range for apatite fission tracks is below 125°C, while that for zircon fission tracks can reach up to 250°C [7-8].

This method is based on the annealing behavior of tracks-generated by the fission of ^{238}U (uranium-238) contained in apatite/zircon-under the influence of temperature over geological time. Most basins have experienced a complex history: they may undergo stable subsidence and sediment accumulation, followed by uplift and erosion, which also complicates the thermal history of sedimentary basins. Since apatite fission tracks contain abundant "thermal

information" and record the entire process of thermal events, this method holds great promise in the study of basin thermal history.

3.2.4. (Uranium-Thorium)/Helium Thermochronology

The principle of the (U-Th)/He dating technique is developed based on the fact that helium (He) is produced by the decay of uranium (U) and thorium (Th) in mineral grains such as apatite. By measuring the contents of radioactive He, U, and Th in a sample, the (U-Th)/He age can be obtained. Minerals applicable for (U-Th)/He thermochronology testing include olivine, pyroxene, amphibole, garnet, apatite, zircon, magnetite, and hematite. Currently, apatite, zircon, and titanite are the most widely used [9]. Based on natural samples and thermal simulation experiments, the closure temperatures of the (U-Th)/He system vary significantly among different minerals: the closure temperature for He diffusion in apatite is relatively low, at 75°C, while that in zircon ranges from 170°C to 190°C [10-12].

Although apatite-based (U-Th)/He thermochronology can be used to study low-temperature cooling history in detail, it must be combined with other paleothermometers (such as apatite fission tracks and vitrinite reflectance) to be effective when applied to the reconstruction of sedimentary basin thermal history.

3.2.5. Fluid Inclusion

A fluid inclusion refers to a substance that is trapped in lattice defects or cavities during the crystallization and growth of minerals by diagenetic and ore-forming fluids, sealed off, and has a phase boundary with the host mineral [13]. It is generally believed that the temperature peak of fluid inclusions should correspond to major tectonic events within the sedimentary basin, and the peak of the highest temperature distribution in the strata represents the period of maximum burial of the basin interior. This serves as a theoretical basis for studying the overall thermal history of a basin using fluid inclusions.

As a paleothermometer, fluid inclusions can effectively determine the temperature at which the host mineral (containing the inclusions) grows or dissolves. Based on this, the geothermal evolution characteristics of the strata can be reconstructed by correlating the temperature peaks of fluid inclusions with their formation stages.

Compared with other paleothermometer methods, fluid inclusions have unique advantages: most currently used paleothermometer methods impose more or less restrictive conditions on samples in different aspects, while inclusions are widely present in minerals-fluid inclusions have relatively the fewest restrictive conditions on samples and are relatively simple to operate. However, not all fluid inclusions in a sample can be used for thermometry; especially for inclusions with small sizes, the measurement accuracy still needs to be improved. Secondly, the correction of pressure for inclusion thermometry is often relatively difficult. Thirdly, the thermal information established based on fluid inclusions is static, which does not fully match the actual development of thermal history.

Since paleothermometer methods can verify simulation results through measured paleothermometer data, they are considered to be highly accurate and practical research methods. However, there is still a lack of effective paleothermometers for reconstructing the thermal history of Early Paleozoic carbonate rock areas in superimposed basins. At present, many scholars have conducted explorations from aspects such as bitumen reflectance, conodont color alteration index (CAI), vitrinite-like body reflectance, bioclastic reflectance, organic free radical concentration, and laser Raman spectroscopy.

3.3. Combination of Tectono-Thermal Evolution Forward Modeling and Paleothermometer Inversion Modeling: Basin Thermal Simulation

The basin-scale paleothermometer method and the lithosphere-scale tectono-thermal evolution method are two independent approaches for studying the basin's dynamic thermal

regime. For sedimentary basins with advanced exploration and research progress, the combination of these two methods provides a new approach to studying basin tectonic evolution through the dynamic thermal regime of sedimentary basins-namely sedimentary basin thermal simulation-which integrates the research of shallow and deep tectono-thermal processes.

The comparison between heat flow histories calculated by different basin models and those inverted by the paleothermometer method is conducive to understanding the genesis and evolution of the basin, thereby revealing the basin's tectonic evolution process. In addition, the thermal simulation results should also be consistent with the deep crustal and lithospheric tectonic data reflected by other geophysical methods such as seismology and gravity, so as to further constrain the basin's tectonic evolution model.

4. Summary

Currently, thermal history reconstruction methods at home and abroad can be categorized into two major types: The first is the forward modeling method for tectono-thermal evolution on the lithospheric scale, also known as the geodynamic method; the second is the paleothermometer inversion modeling method on the basin scale, which mainly includes four approaches: fitting calculation of basin paleogeotemperature (stochastic inversion), basin thermal evolution history (paleogeothermal gradient method), thermal flow history at the basin bottom (paleo-heat flow history), and apatite fission track method. The combination of tectono-thermal evolution forward modeling and paleothermometer inversion modeling provides a new approach for studying tectonic evolution through the dynamic thermal regime of sedimentary basins-namely sedimentary basin thermal simulation-which integrates the research of shallow and deep tectono-thermal processes.

The paleothermometer method uses paleothermometers to invert the thermal history of strata and the heat flow at the basin bottom. Its main approaches include vitrinite reflectance (Ro), vitrinite reflectance gradient, apatite fission track, EASY%Ro method, conodont color alteration index (CAI), authigenic mineral assemblage, fluid inclusion thermometry, oxygen isotope analysis, and $^{40}\text{Ar}/^{39}\text{Ar}$ dating.

The application of various thermal history analysis methods in basin research is becoming increasingly in-depth. Fission track and vitrinite reflectance have become and will continue to be the mainstream methods in basin thermal history research. Meanwhile, the basin thermal simulation method-a new approach for studying paleogeotemperature by combining basin tectono-thermal evolution models with organic matter maturity fitting calculations-is also gradually developing. Only by comprehensively comparing various basin thermal history research methods and fully considering the influencing factors of thermal history can the basin's thermal evolution history be accurately reconstructed.

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