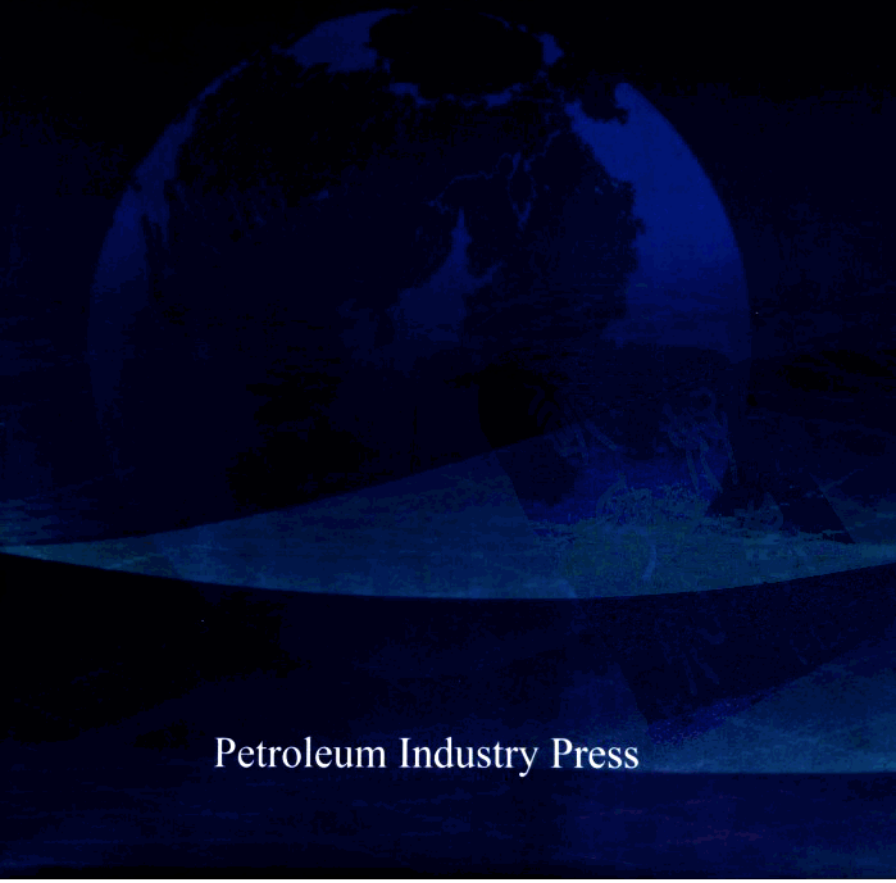
Numerical Methods of Petroliferous Basin Modeling

Third Edition

Shi Guangren



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Abstract

Numerical simulation of petroliferous basins is a new technology developed in the past 25 years. Based on petroleum geological mechanism, it applies multi-disciplinary knowledge to quantitatively simulate geohistory, geothermal history, hydrocarbon generation history, hydrocarbon expulsion history and hydrocarbon migration-accumulation history of an exploration area such as a basin, depression, sag and secondary sag so as to make an integrated evaluation and to indicate a favorable play for exploration.

This book contains the introduction, the generality of basin modeling system, the principles, methods and applications of five models of geohistory, geothermal history (including diagenetic history), hydrocarbon generation history, hydrocarbon expulsion history and hydrocarbon migration-accumulation history, the parameter sensitivity and risk analyses of basin modeling, the integrated analysis and evaluation on petroleum resources, as well as the basin modeling software technology. In addition, the related exercises are attached in the end of each chapter from Chapter 1 to Chapter 10, and the answers to them are totally given in the end of the book.

The book could be used as a textbook of undergraduate and graduate students majoring in petroleum geology, and also used by the scientists and engineers in the field of petroleum geology.

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Preface

The book of "Numerical Methods of Petroliferous Basin Modeling", written by Prof. Shi Guangren, is an aggregation of principle, method, software technology and application and also a monograph to introduce the numerical methods of petroliferous basin modeling across-the-board.

Basin modeling is a new technology developed in the past 25 years. Based on physical and chemical mechanism of petroleum geology, it quantitatively simulates the evolution history of petroleum geology of a petroliferous basin by applying multiple disciplines, thus correctly establishing geological and reservoir models, which plays an important role in the guidance to petroleum exploration. This is a rising subject in the field of petroleum geology science in the present world.

The book is a compendium of ideas gained by the author over 20 years from the research, teaching and application of basin modeling and from the references of a great deal of related literatures published in China and overseas. It reflects the highest level of quantitative study on petroleum geology of a petroliferous basin. The book presents the principles, methods and case studies of five models of geohistory, geothermal history (including diagenetic history), hydrocarbon generation history, hydrocarbon expulsion history, hydrocarbon migration-accumulation history, and the parameter sensitivity and risk analyses in the light of the concept of hydrocarbon generation from organic matters in a petroliferous basin. For each model, the book not only describes the advanced methods that are commonly used in China and abroad, but also introduces some effective methods that the author has originally created and improved. All these enrich and perfect the theory and methods of the numerical simulation of a petroliferous basin, creating an integrated and sophisticated system both theoretically and technologically, and then greatly promoting the numerical simulation of petroliferous basins.

The book is characterized by the combination of theory with practice. It focuses on the elaboration of methods and techniques, explains the principles and methods in a simple way and derives the formulas strictly and accurately. The most methods presented in the book are proved to be effective in the practice and available in the software application. In a word, readers can either learn the principles, methods and applications of the basin modeling from the macroscopic view or master all the methods from the microscopic view so that they can develop and apply the basin modeling software based on the specific geological conditions and reservoir types. Meanwhile, they can conduct a further study to improve the success rate for exploration.

In the recent years, there are few books covering the technologies of basin modeling in China and abroad. Most the like published only expounds the method of quantitative simula-

tion of a subject or introduces a general theory of a specific subject. There is no such a monograph that presents the technology of basin modeling in all round and systematic way. Currently, the numerical method of a petroliferous basin modeling is turning into a conventional tool for the study of petroleum geology and an integrated method for petroleum exploration. In this case, this book is a scarce reference book for teaching and scientific research. The publication of the book will definitely promote the development of basin modeling technology and petroleum exploration.

Prof. Zhai Guangming (Member of the Chinese Academy of Engineering)
August 12, 2004

Foreword

This book is a compendium of ideas that the author gained over 20 years of study, teaching and application of the basin modeling. The author tries to write into the book the more advanced, effective and proof techniques as possible.

The author tried to explain the principles, methods and applications of the basin modeling in a simple way that readers not only can understand from the macroscopic view but also can master the details of all kinds of techniques from the microscopic view so that they are in a position to develop the software themselves.

The first edition of "Numerical Methods of Petroliferous Basin Modeling" was published by the Petroleum Industry Press in August 1994. The second edition of the book was published by the press in March, 1999, in which the major new contents are: backstripping considering as more geological phenomena as possible, tectonic subsidence and balanced cross section in geohistory model; algorithm with the known geothermal gradient history, algorithm with the known heatflow history and statistics method to estimate present heatflow in geothermal history model; Easy R_o and calculation of Total Organic Carbon (TOC) in hydrocarbon generation history model; mass balance method for gas expulsion in hydrocarbon expulsion history model; present fluid potential of 3-phase (water, oil, gas), simplified method of 2-D (x, y) and 2-phase (oil, gas) and discussion of simulation method and algorithm in hydrocarbon migration-accumulation history model; and integrated analysis and evaluation on petroleum resources.

This book is the third edition. Besides the revision and renewal on each part of the second edition to some extent, it provides some major new contents of diagenetic history including smectite to illite transformation and quartz cementation in geothermal history model; isomerization index of sterane and hopane in hydrocarbon generation history model; compaction-filtration method for oil expulsion and pressure-difference-filtration method for oil expulsion in hydrocarbon expulsion history model; finite volume of 3-D (x, y, z) and 3-phase (water, oil, gas) history simulation in hydrocarbon migration-accumulation history model; parameter sensitivity and risk analyses of basin modeling; in addition, related exercises are attached in each end of Chapter 1 to Chapter 10, and the answers to them are totally given in the end of the book.

The book lists all the quotations from other literatures or works that the reader can take them as reference in references or documents of this book.

I wish to acknowledge the instruction and support of Prof. Zhai Guangming, a member of the Chinese Academy of Engineering, in the computer applications in petroleum geology, and also the support and help of the computer application technology department of the RIPED in my method study and software development of basin modeling. The third edition of the book is partly sponsored by the department.

This book corresponds with the third edition book in Chinese, which is translated from

Chinese to English by the author himself and revised by a specialist of English in China.

Since the first English edition of this book was published in 2000, the author has delivered a series of English lectures on basin modeling to graduate students by taking the book as a textbook.

Shi Guangren
April 5, 2005

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Chapter 1 Introduction

The field of petroleum geology is still in a qualitative or partly quantitative stage due to the hybrid-discipline and complexity of petroleum geology. The computer applications in petroleum geology fall in three major categories: modeling technology, statistic technology and expert system. The modeling technology is based on physical and chemical mechanism of petroleum geology, and has been developed for almost 25 years; the statistic technology is based on the statistic analysis to the geological data, and has been developed for almost 40 years; and the expert system is based on the artificial intelligence of geologists' insights, and has been developed for almost 25 years. Those three technologies are different, and each has its strong points and each has its weak points. However, from the geological mechanism point of view, the modeling technology is much better than the other two, because it can directly expose the regularity of oil and gas in a basin.

Basin modeling is used to quantitatively simulate the formation and evolution of a petroliferous basin in space-time together with the generation, migration and accumulation of hydrocarbons by setting up a geological model followed by a mathematical model and subsequently the creation of computer software for numerical simulation on the basis of physical and chemical principles of petroleum geology. Therefore, it can be defined as "Basin Numerical Simulation" from scientific classification; and it can also be defined as "Basin Modeling System" from its software product. This is a rising subject appearing in the field of petroleum geology in the present world.

Basin modeling technology has grown for almost 25 years; however, it is still the technology that is being developed for petroleum exploration and also a very active resort of quantitative study on petroleum geology. Basin modeling is not only a tool for the evaluation of petroleum resources, but also a necessary technology for the geological analysis of petroleum exploration.

1 Objectives and Description of Basin Modeling

The work that geologists undertake is to find more and larger hydrocarbon reservoirs in a faster way but with less investment and to confirm the subsurface petroleum resources so as to lay the material foundation for the development of petroleum industry at high speed. But the natural conditions to control the hydrocarbon distribution are very complicated since oil and gas occur underground and appear as fluid. Then, what are the conditions to control their occurrence? How to look for hydrocarbon reservoirs? This is the prime question that the petroleum geologists should answer (Zhang and Zhang, 1989; Zhai *et al.*, 1995; Dai, 1997; Dai *et al.*, 2000, 2003; Li and Li, 2003). The task of basin modeling is to lead the petroleum geology research to quantification and computerization, to provide petroleum geologists with a faster, quantitative and integrated research means, that is basin modeling sys-

tem. The method of basin modeling comes from the conventional petroleum geological research, but is different from this kind of research, i. e. full quantification. Basin modeling system, a large and integrated software established based on petroleum geology and by utilizing the knowledge from hybrid disciplines, consists of five models of geohistory, geothermal history, hydrocarbon generation history, hydrocarbon expulsion history and hydrocarbon migration-accumulation history, which cover almost all the branches of petroleum geology. The quantitative simulation of history is able to reveal the regularity of oil and gas in the basin, not only to improve the research method on petroleum geology, but also to make computer mapping replace manual mapping. That is why some scholars refer it as a revolution in petroleum geology.

Since the geological process of petroleum is very long and complex as well as the left imprints that could be field-measured are rare and localized, it brings great difficulties to quantitative study on petroleum geology. The rapid development of oilfield prospecting and experiment technology in 1980's enables to acquire large amount of data that had never been obtained before, and promote the advances of the theory of petroleum geology and the high development of mathematical geology in 1990's. This is reflected by the prevalent applications of basin numerical modeling and the winning completion of the 1st, 2nd and 3rd national assessment of petroleum resources in China. Mathematical geology, therefore, sets up its own position in petroleum geology and becomes an independent branch subject in petroleum geology.

Now the computer application to the field of petroleum geology is still an unsubstantial part in petroleum exploration and production, which does not coincide with the important position of petroleum geology in petroleum exploration and production. This situation is being changed by the new technology of basin modeling to make the quantification, computerization and mapping automatization in petroleum geology. It has been approved by the practice that basin modeling is one of the important ways to make petroleum geology quantification.

2 Basin Modeling Scope

Basin modeling, as its name implies, is designed to make historical simulation to the evolution of the whole basin. As a matter of fact, however, so long as it is a basically independent hydrocarbon generation-accumulation unit (i. e. Petroleum System), the simulation can be made on it. So the area to be studied may be a basin, depression, sag, or secondary sag. On entering the data of geology, seismic, logging, geochemistry, even data from production laboratory, basin modeling system simulates depositional history, structural history, heatflow history, temperature history, diagenetic history, hydrocarbon generation history, hydrocarbon expulsion history and hydrocarbon migration-accumulation history, thus making integrated analysis and evaluation on petroleum resources to indicate the favorable play for exploration.

The embryo basin modeling is based on the theory of organic hydrocarbon generation, within the confinement of the calculation of the amount of hydrocarbons generated. The early basin modeling system in 1980's consists of three models of geohistory, geothermal history and hydrocarbon generation history, whereas the basin modeling system since 1990's con-

tains five models of geohistory, geothermal history (including diagenetic history), hydrocarbon generation history, hydrocarbon expulsion history and hydrocarbon migration-accumulation history. A basin modeling system in China also has a platform of integrated analysis by combining "basin modeling results", "other geological information" and "geologists' insights".

A complete basin modeling system consists of the following five models:

——Geohistory

——Geothermal history (including diagenetic history)

——Hydrocarbon generation history

——Hydrocarbon expulsion history (primary migration)

——Hydrocarbon migration-accumulation history (secondary migration)

The function of geohistory model is to rebuild the depositional and structural histories of a petroliferous basin. The following phenomena should be taken into account: depositional hiatus, sedimentary compaction, undercompaction (overpressure), single-formation erosion, multi-formation continuous erosion, fault and paleo-bathymetry etc. Geohistory model is the basis of basin modeling, so the accuracy of this model directly affects the rest four models. Three kinds of method are used: backstripping (to normal-compacted formations), overpressure (to under-compacted formations), and the combined method of backstripping and overpressure (to normal-compacted and/or under-compacted formations). These three kinds of method are available on the assumption of vertical subsidence. It is suggested to apply the technique of balanced cross section (to tension and compression of the basin) if the assumption is to be knocked down.

The function of geothermal history model is to rebuild the heatflow, temperature and diagenetic histories of a petroliferous basin. The geothermal history model is a critical link in basin modeling since temperature evolution is the most important factor in hydrocarbon maturity. Two kinds of method are employed: geothermics that is less reliable, the combined method of geothermics and geochemistry that is more reliable. Based on the simulation results of geohistory and geothermal history, it is possible to calculate the diagenetic history, i. e. smectite to illite transformation and quartz cementation. The smectite to illite transformation results in the change of lithology while the quartz cementation affects the development history of porosity.

The function of hydrocarbon generation history model is to rebuild the hydrocarbon maturity and hydrocarbon yield histories of a petroliferous basin. This model is an important part in basin modeling, because hydrocarbon yield history is one part of petroleum resource evaluation. Three kinds of method are utilized: $TTI-R_o$ that is applicable to an area in more explored stage (i. e. there exist more wells drilled and seismic sections), Kinetic Equations that is applicable to an area in moderate explored stage (i. e. there exist some wells drilled and seismic sections), and Easy R_o that is applicable to an area in less explored stage (i. e. there exist only a few wells drilled).

The function of hydrocarbon expulsion history model is to rebuild the hydrocarbon expulsion history of a petroliferous basin (primary migration). The model lies in a very important position in basin modeling, because the history of hydrocarbon expulsion and direction is one part of petroleum resource evaluation. Four kinds of method are employed: the compaction-filtration is to study the expulsion of oil, which is not only applicable to the normal-

compacted formations where the curve of porosity versus depth is normal, but also to the under-compacted formations where the curve of porosity versus depth is abnormal (porosity varies little with depth or even does not); the pressure-difference-filtration is to study the expulsion of oil, which is applicable to the under-compacted formations where the curve of porosity versus depth is abnormal (porosity varies little with depth or even does not); the mass balance is to study the expulsion of gas; and the mechanics of fluid flow through porous media is to study the expulsions of oil, gas and water.

The function of hydrocarbon migration-accumulation history model is to rebuild the hydrocarbon migration-accumulation history of a petroliferous basin (secondary migration). This model is the most important part in basin modeling, because hydrocarbon migration-accumulation history is the most important part in petroleum resource evaluation. Four kinds of method are employed: the present fluid potential of 3-phase (water, oil, gas) is applicable to the case of pool-forming at the late stage or the middle stage but no violent tectonic movement at late stage; the simplified method of pseudo 3-D (x, y, *formation thickness*) and 2-phase (oil, gas) is applicable to pool-forming at every stage; the finite difference of 2-D (x, z) and 3-phase (water, oil, gas) is applicable to pool-forming at every stage, its simulation results depend on the perfection and accuracy of known parameters since the 3-phase fluid flow on cross section and the complexity of whole problem; and the finite volume of 3-D (x, y, z) and 3-phase (water, oil, gas) is applicable to pool-forming at every stage, its simulation results also depend on the perfection and accuracy of known parameters since the 3-phase fluid flow in 3-D space and the complexity of whole problem.

Primary migration mainly occurs in the vertical direction, and can be simulated by a one-dimensional model. Secondary migration not only happens in the vertical direction, but also in the lateral direction mainly. So it is required to use a two-dimensional (x, y or x, z) at least, and ideally a three-dimensional system (x, y, z) in order to simulate secondary migration adequately. Obviously, a 1-D system can only involve the first four models, while the other two systems can include the above-mentioned five models. The presently used basin modeling system is still the 1-D and 2-D systems. The 2-D and 3-D systems need more data than 1-D system, but they can simulate hydrocarbon secondary migration.

The function of integrated analysis and evaluation on petroleum resources is to delineate the location of hydrocarbon reservoirs and provide corresponding accumulation estimates. The technique of integrated evaluation is to introduce the traditional method of petroleum geology on the basis of basin modeling. To an area to be studied, "basin modeling results", "other geological information" and "geologists' insights" should be combined together. The interactive function of computer makes it possible to combine the above-mentioned three components, which makes up for the weakness of unicity of the basin modeling in the study of petroleum geology, and also overcomes the shortcomings of qualitative or semi-quantitative analysis of the traditional geological study. In a word, this technique succeeds the advantages of the comprehensive analysis that the traditional geological study possesses and absorbs the merits of the quantitative analysis that basin modeling has, which brings about a big leap to the technological level of petroleum resource evaluation and petroleum geological analysis.

Basin modeling has used deterministic model since 1980's, i. e. input parameters are u-

nique while modeling results unique, whereas the other quantitative tools (Monte Carlo) of resource assessment use the risk model. Due to the complexity of subsurface petroleum-geological conditions and the limitation of people's understandings, the parameters used by basin modeling have some uncertainties, resulting in the risks of modeling results. The main reason why basin modeling has not been changed to the risk model for many years is that categories of parameters are various and large computer time is consumed. In the resent years, a few scholars commenced studying on the parameter sensitivity and risk analyses of basin modeling so as to make basin modeling change from deterministic model to risk model, attaining the effect that can match with other quantitative tools (Monte Carlo) of resource assessment.

Generally speaking, the advantages and disadvantages of a basin modeling system can be identified from the following: **a)** it inputs the maximum types and amounts of parameters; **b)** the 1-D system should consist of the above-mentioned first four models while 2-D and 3-D systems consist of five models; **c)** the methods that each model uses should be correct and the techniques advanced; **d)** it outputs all types of map and they are practical and accurate; **e)** it should have the functions of technique for the petroleum resource evaluation and integrated analysis; and **f)** it should have the functions of parameter sensitivity and risk analyses as possible.

3 Development History of Basin Modeling

Basin modeling is a new large and integrated subject studied in the field of petroleum geology in the present world. 1980's were the test application stage of basin modeling, whereas 1990's the stage of practical application. The success of application made it become the most content-rich and most beneficial quantitative research tool in petroleum geology. The essential factor of the success is the correct physical and chemical mechanism of the petroleum-geological processes. For instance, geohistory model, considering as more geological phenomena as possible, i. e. depositional hiatus, sedimentary compaction, undercompaction (overpressure), single-formation erosion, multi-formation continuous erosion, fault and paleo-bathymetry etc., rebuilds the depositional and structural histories of a petroliferous basin more accurately; geothermal history model, taking heat conduction, convection and radiation into account, and using the inverse deduction with the restraint of geochemical data, rebuilds the heatflow, temperature and diagenetic histories of the basin more accurately; hydrocarbon generation history model, making use of the multiple geochemical indexes for expressing the hydrocarbon maturity and source rocks (shale, carbonate and coal) based on the experiment of thermal degradation of kerogens, rebuilds the hydrocarbon maturity and hydrocarbon yield histories of the basin more accurately; hydrocarbon expulsion history model, using the compaction-filtration or pressure-difference-filtration to study the expulsion of oil, and the mass balance to study the expulsion of gas, rebuilds the history of the amount of expelled hydrocarbons of the basin basically and more accurately to a certain extent; and hydrocarbon migration-accumulation history model, using the mechanics of fluid flow through porous media, and considering the driving forces of fluid potential, buoyancy and capillary pressure etc. as well as the migration channel factors of lithology, fault and unconformity etc., rebuilds the

hydrocarbon migration-accumulation history of the basin basically and more accurately to a certain extent.

A large amount of study has been conducted in some countries for almost 25 years and greater progress has been made. For instance, basin modeling systems on different scale have been set up on computers and gone on stream in Germany (Yükler *et al.*, 1978; Welte and Yükler, 1981; Tissot and Welte, 1984), France (Tissot and Welte, 1984; Ungerer *et al.*, 1984, 1990; Forbes *et al.*, 1991), U. S. A. (Waples, 1980, 1998; Lerche *et al.*, 1984; Lerche, 1988a, 1988b, 1990, 1992; Sweeney and Burnham, 1990; Waples *et al.*, 1992a, 1992b; Sweeney *et al.*, 1995; Chen *et al.*, 2002; Leonard, 2003), UK (England *et al.*, 1987; Pepper and Corvi, 1995a, 1995c; Pepper and Dodd, 1995b; Scheichl *et al.*, 2003), Japan (Nakayama and Van Siclen, 1981; Nakayama, 1987; Nakayama and Lerche, 1987; Nakayama, 1988; Okui *et al.*, 1998) and China (Shi and Kuo, 1988a, 1988b; Shi, 1989, 1994, 1996, 1999a, 2000, 2001, 2002, 2003; Shi *et al.*, 1989, 1992, 1993, 1996a, 1996b, 1996c, 1997a, 1997b, 1998, 2002b, 2002c, 2003a; Feng and Shi, 1989; Pang *et al.*, 1993; Mi *et al.*, 1994; Liu *et al.*, 1994; Guo *et al.*, 1998; Feng *et al.*, 2001; Pang and Chen, 2003; Shi and Zhang, 2003b, 2004a, 2004b, 2004c) etc. In the first 10 years, the 1-D system was dominated, focusing on the study of geohistory, geothermal history and hydrocarbon generation history, most of which were in the stage of test application; while in the latter 15 years, 2-D system was dominated, focusing on the study of hydrocarbon expulsion history and hydrocarbon migration-accumulation history in the stage of practical application.

3.1 History of Basin Modeling Development in the World

The history of basin modeling development in the world will be described as follows in the order of countries and time according to the published literatures:

In 1978, the Integrated Exploration Systems (hereafter refer to as "IES") in Germany established the first 1-D basin modeling system in the world (Yükler *et al.*, 1978; Welte and Yükler, 1981). It was designed to derive fluid velocity in the under-compacted formations with overpressure equation, providing the parameters for the calculation of convection in the heatflow equation; to calculate temperature history with the heatflow equation of thermal conductivity and convection; to repeatedly adjust the calculation in order to make the calculated results agree with the actual data, so as to obtain the final results including burial history; to evaluate TTI and R_o by combining burial history and temperature history; and to calculate the amount of generated hydrocarbons and the amount of expelled hydrocarbons based on R_o. Since this is a 1-D system, it is unable to simulate hydrocarbon secondary migration and accumulation.

In 1984, the Institute of French Petroleum (hereafter refer to as "IFP") in France established a more completed 2-D basin modeling system (Ungerer *et al.*, 1984, 1990). It was designed to calculate burial history with backstripping by entering the data of interpreted logging and seismic section; to calculate heatflow history with geodynamics by entering the data of seismic refraction and measured present heatflow; to calculate temperature history and hydrocarbon maturity history with the method of geothermics and hydrocarbon maturity by entering the data of lithology and thermal conductivity; to calculate fluid pressure history and oil accumulation history with the method of 2-phase migration by entering the data of