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Recent developments in petroleum geochemistry

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Abstract: Although steady progress has been made in traditional petroleum geochemistry, no recent advances are comparable to the most-important developments of the last thirty years. Biomarkers, kinetics of thermal indicators and of hydrocarbon generation and cracking, and carbon-isotope-ratio gc-ms are the most exciting research areas today. In addition, application of traditional petroleum geochemistry to reservoir problems has opened the door to intriguing new areas for interdisciplinary investigations.

Much of the most interesting activity in the field of geochemistry currently is directed toward basin modeling. Inclusion of basin modeling as a subdiscipline of geochemistry is a historical quirk that has exerted some not entirely salutary control on the direction of research and development of basin models. Future work in basin modeling should attempt to address geological and geophysical problems that have until now been given short shrift.

Weaknesses in current basin models include scientific limitations, computer limitations, and inadequate applications. Solving these problems will require major efforts by groups who understand the goals and needs of exploration and can build a model that can be used easily by exploration personnel. Proper training in both the technology and philosophy of modeling are of paramount importance. It is not yet clear how thoroughly basin modeling will be adopted for routine exploration work; success will depend largely on the skill with which modeling technology is transferred from research laboratories to exploration units.

INTRODUCTION

Petroleum geochemistry has now existed as a distinct discipline for more than thirty years. Tremendous progress has been made during that time in understanding and quantifying the various processes contributing to preservation of organic matter, formation and thermal transformation of kerogen, hydrocarbon generation and cracking, and expulsion and migration. As in all branches of science, there have been two kinds of progress in geochemistry: relatively slow, conservative progress as the ramifications of individual problems were thoroughly considered, and rapid progress and the development of entirely new subdisciplines following the advent of new technologies or ways of thinking.

In order to gain a proper perspective on the present status of petroleum geochemistry, it is necessary to view current developments against a backdrop of the major events in its history. Any list of "major" events is necessarily

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Keynote address at GSM Petroleum Geology Seminar 1990 subjective, but most workers would probably agree that the events shown in Table 1 were of great importance.

Table 1: Major events in the history of petroleum geochemistry

about 1960	recognition that compostions of rock extracts were related to maturity
1960's	recognition that compositions of rock extracts and crude oils were related to nature of the source material
late 1960'a	application of palynology to determine kerogen maturity through spore color
early 1970's	application of vitrinite reflectance to kerogens as an "objective" maturity indicator
late 1970's	development of Rock-Eval and routine application in source-rock evaluation
early 1980's	popularization of maturity modeling
early 1980's	popularization of biomarkers as useful tools for interpreting organic facies and maturity, and for oil-source rock and oil-oil correlations

However, Table 1 does not show any first-magnitude events over the last few years. Recent progress, therefore, appears to be incremental rather than of the quantum-leap variety. However, several years from now we may find that certain current developments in petroleum geochemistry were actually more revolutionary than evolutionary. I will mention these briefly below.

Moreover, petroleum geochemistry is rapidly broadening and becoming more interdisciplinary: for example, applications of geochemistry to reservoir studies and to basin modeling are now becoming popular. These nontraditional applications of geochemistry actually represent some of the most interesting future potential, and will also be discussed in detail.

IMPORTANT DEVELOPMENTS IN TRADITIONAL PETROLEUM GEOCHEMISTRY

Kinetics

Hydrocarbon generation and cracking

Kinetic models for hydrocarbon generation and cracking, first published more than two decades ago (Tissot, 1969), are slowly but surely replacing the TTI method (Lopatin, 1971; Waples, 1980). Recent kinetic models (e.g., Tissot *et al.*, 1987; Espitalié *et al.*, 1988; Burnham and Braun, 1990) are highly sophisticated and seem to reproduce well the behavior of kerogens during both laboratory pyrolysis and natural subsurface heating. The change from dominance by TTI models to dominance by kinetic models is welcome, because kinetic models are technically better, and because kinetic models can consider variations in kerogen type more accurately than can TTI models. In addition to (or instead of) using the traditional type I, II, and III kerogens, some workers today determine kinetic parameters for individual kerogen types (e.g., Tissot *et al.*, 1987; Burnham and Braun, 1990; Hunt *et al.*, 1991; Waples, in press a). We are finding that dividing kerogens into three simple endmember types (and mixtures of those end members) is an inadequate way to describe the diversity of organic matter and the biological systems that have produced and transformed it through geologic history and around the globe. The trend toward "personalized" kinetic descriptions of individual samples or source units will probably gain popularity in the future (Fig. 1).

Little progress has been made in deriving reliable kinetics for cracking of oils, although some data are now available on high-sulfur oils as well as normal oils (Behar *et al.*, 1988). However, I expect additional data to be published in the next couple of years, as cracking finally receives the attention it deserves.

Thermal indicators

The other important application of kinetics in petroleum geochemistry today is for describing changes in thermal indicators. It is important to have reliable kinetic descriptions of transformations of a variety of thermal indicators, because use of multiple thermal indicators provides information necessary for accurately reconstructing burial and thermal histories. These histories in turn are necessary for maturity modeling and basin modeling. Multiple indicators are necessary because in any given case one or more of the available indicators may not work well, and because each indicator gives a slightly different perspective on the total thermal history (Waples, in press a).

The most-reliable kinetic data are probably those for vitrinite reflectance (Burnham and Sweeney, 1989; Sweeney and Burnham, 1990). Kinetic descriptions of Tmax (Sweeney, 1990) are less secure. Apatite fission-track annealing has been described kinetically for several years, but considerable controversy surrounds this technology (see Naeser, in press; Crowley *et al.*, in press). Ritter *et al.* (in press) have recently derived preliminary kinetic parameters for a variety of new indicators. Alexander *et al.* (1990, 1991) have developed kinetic descriptions of biphenyl transformations and ester elimination from kerogen, and have tested them successfully against empirical data, but have not published details.

Among the earliest thermal indicators to be described kinetically were biomarker transformations such as sterane and hopane epimerization and

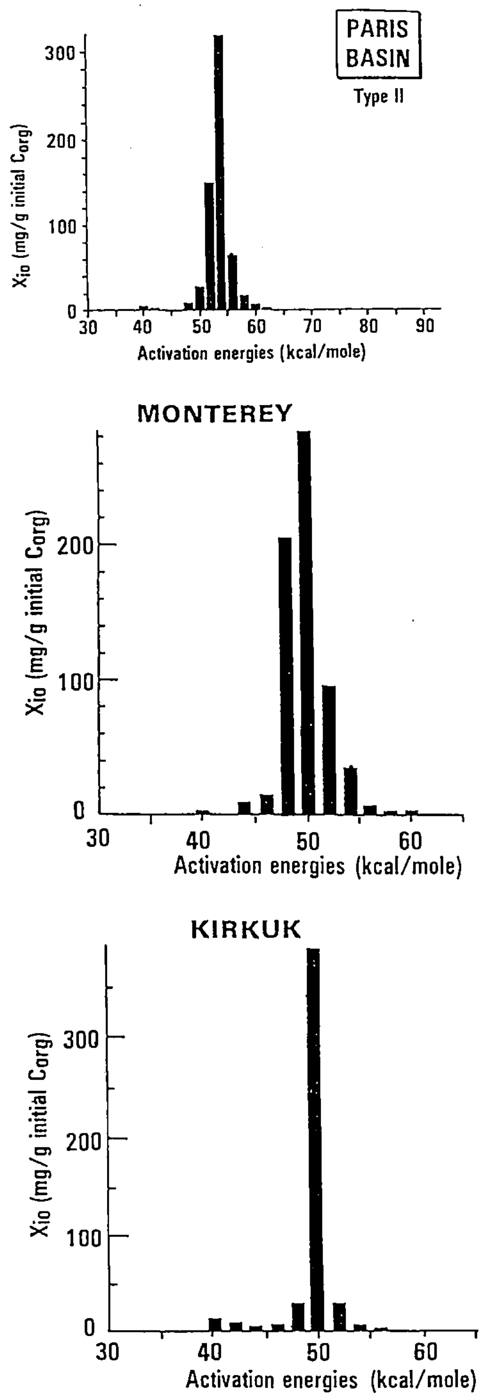

Figure 1: Activation energies for three type II kerogens presented in histogram form. Top: standard type II kerogen from the Toarcian of the Paris Basin. Middle: high-sulfur type II kerogen (type II-S) from the Monterey Formation of California. Bottom: type II-S kerogen from Iraq. Values on the y-axis represent frequency of occurrence of bonds with each activation energy. Total number of breakable bonds depends on oil-generative potential of the kerogen. Activation energies for the type II-S kerogens are on the everage about 4 kcal mol less than that for standard type II kerogen. From Tissot *et al.*, 1987; reprinted with permission of the American Association of Petroleum Geologists.

sterane aromatization (e.g., Mackenzie, 1984). However, recent work (e.g., Abbott *et al.*, 1990) suggests that the chemical processes involved in such reactions are probably more complex than originally thought, and that the existing kinetic descriptions may not be correct. The future may bring considerable rethinking of the problem of biomarker kinetics, and could herald a greater role for calibration of biomarker kinetics with empirical field data instead of with data from laboratory simulations.

Biomarkers

Both good news and bad news are emerging from recent research on biomarkers. The bad news is that biomarker reactions during both diagenesis and catagenesis are more complicated than was originally thought. Therefore, biomarker kinetics, as mentioned above, are in question today. Moreover, specific precursor-product relationships in thermal transformations may not be as straightforward as was once believed.

Some of the older rules for interpreting the presence, absence, or relative amounts of certain biomarkers in terms of organic facies have also been extensively rewritten. Gammacerane, for example, is now seen more as an indicator of abnormal salinity than of lacustrine environments, as was previously believed (e.g., ten Haven *et al.*, 1987; Brassell *et al.*, 1988). Other examples of uncertainty in current applications of steranes and triterpanes to organic-facies interpretations are discussed in Waples and Machihara (1990, 1991).

The good news is the frequent reporting of new biomarkers, some of which appear to be associated with certain unusual facies (Table 2). When viewed as assemblages in the way that microfossils are, and when fully integrated with geological information, biomarkers will become increasingly valuable in interpreting depositional and diagenetic conditions and for correlation studies.

Table 2: New biomarkers useful as facies indicators

Name	Environment	Source	Ref.
Bicadinanes	Tertiary swamps of SE Asia	*Dipterocarpaceae* (land plants containing dammar resin)	(1)
Hexacyclic hopanoids	Evaporites	?	(2)
Extended tricyclic triterpanes (up to C_{41})	Lacustrine black shales	prokaryotes	(3)
Ring-A methylated 28, 30-bisnorhopane	Anoxic marine black shales	prokaryotes (?)	(4)

References are (1) Alam and Pearson, 1990; (2) Connan and Dessort, 1987; (3) Kruge *et al.*, 1990; (4) Farrimond *et al.*, 1990.

Carbon-isotope-ratio GC/MS

There have been sporadic reports in the literature of carbon-isotope ratios measured on individual compounds (e.g., Welte, 1969; Vogler *et al.*, 1981). Nevertheless, in spite of the obvious potential value of such data, such ratios have seldom been used because of technical difficulties in obtaining enough material to carry out the measurements. Recently, however, a new instrument has been developed to perform gas-chromatographic separations of complex mixtures and then measure carbon-isotope ratios automatically on individual compounds.

Initial results are extremely interesting. For example, Freeman *et al.* (1990) measured carbon-isotope ratios of 21 different peaks in a gas chromatogram of saturated hydrocarbons in a Messel Shale extract. Among the fascinating observations were:

1. two acyclic isoprenoids and the C_{29} hopane all had highly negative $\delta^{13}C$ values (–60 to –73 ‰) suggesting they were formed by methanogens;
2. C_{30} and C_{31} hopanes $\delta^{13}C$ values near –35 to –40 ‰, indicative of a common (but nonmethaogen) origin; and
3. pristane and phytane differed from each other (–25 ‰ and –32 ‰, respectively), suggesting different sources.

I anticipate that gc/isotope-ratio-ms instruments will soon become indispensible for molecular geochemists. They may well revolutionize our understanding of the relative importances of original organic matter compared to diagenetically produced organic matter in forming kerogen. If so, this technology will play a major future role in organic-facies and correlation studies.

RECENT DEVELOPMENTS IN NONTRADITIONAL PETROLEUM GEOCHEMISTRY

Reservoir geochemistry

Until recently, virtually all applications of petroleum geochemistry had been to exploration problems. Now, however, some attention is turning to studying the existence and causes of geochemical variation within oil reservoirs. England (1990) and Horstad *et al.* (1990) have discussed processes which lead to segregation (e.g., preferential permeability pathways, sourcing from different directions) and mixing (convection, diffusion) of oils of different original compositions, as well as processes like biodegradation that transform gross oil composition in reservoirs. They have then documented these trends and processes using both gross and detailed-molecular compositions as tracers.

The expansion of petroleum geochemistry into reservoir studies is very healthy and important, because it will promote more integration of geochemical and geological concepts in describing fluid flow, and will undoubtedly lead to a clearer understanding of migration in general. Furthermore, it is consistent with growing interest in the petroleum industry in finding more efficient ways to produce the reserves we have already located, rather than simply in searching for new fields. Finally, it will provide new stimulus for creative thinking in geochemistry by encouraging collaboration among geochemists, geologists, and reservoir engineers.

Basin modeling

Introduction

Basin modeling (e.g., Ungerer *et al.*, 1990) has rather consistently been considered as a nontraditional branch of petroleum geochemistry. The rationale for this decision is fairly straightforward: (1) in basin modeling we are mainly concerned with the hydrocarbons in the basin (see Waples, in press b; Hermanrud, in press), and (2) maturity modeling has formed the heart and core of most basin models. However, the classification of basin modeling as a branch of geochemistry is in my opinion erroneous, and has led to mistaken emphasis in research, development, and application of basin models.

In particular, the emphasis on geochemistry has led to underevaluation of the importance of geology and geophysics in basin models and in basin modeling. Some of these errors are now beginning to be corrected, however, as attention shifts from the relatively simple and well-understood problems of kinetics of kerogen transformation, toward more difficult and perhaps more important unsolved problems related to expulsion, migration, heat flow, petrophysical properties, the role of faults and fractures, sensitivity analysis, and other vital components of basin models.

Because of its historical link to maturity models and geochemistry, and because it is designed to be applied in exploration, basin modeling provides an excellent opportunity for geochemists to make a substantive contribution to exploration. However, there is still considerable skepticism in some quarters about the value of basin modeling for exploration. Some geologists believe modeling is only of value when one has few data, because if data are abundant, one doesn't need a model. Others argue to the contrary, that modeling is only of value when data are abundant, because without data to constrain one's ideas, one can construct and justify any scenario one wishes.

I would argue that properly executed modeling is of value at all stages of exploration, although one's methods, objectives, and expectations must change as data density and quality change. In frontier areas there is considerable uncertainty in all input data, but systematically deriving a coherent geologic model that agrees with all available data is better than guessing. In wellexplored areas, in contrast, where the input data for the basin model will often be well constrained and where the output is therefore not much of a surprise, the main value of modeling may lie in showing timing of generation and migration, and in suggesting new ideas that can be pursued (e.g., new areas into which hydrocarbon migration may have occurred). Properly used, models should stimulate thinking as well as provide answers. Numerical answers may be in error because of faulty input data, but stimulating one's thinking is never a waste.

Unfortunately, all existing basin models have significant weaknesses. These weakness can be divided into three groups: limitations or errors in the scientific concepts; limitations in the computer codes that use these scientific concepts; and poor applications. Understanding and correcting (or compensating for) these weaknesses is vitally important for high-quality basin modeling.

Scientific weaknesses

The errors in scientific concepts are more errors of omission than of commission. In other words, existing basin models are far from complete. I fault overemphasis on safe research on well-understood problems such as kinetics of hydrocarbon generation at the expense of more important but more difficult topics. The areas which have received the most attention are mainly geochemical, reflecting the interests and expertise of the researchers doing the work; those which have been ignored are much more petrophysical in nature. The best way to change research emphasis would probably be to bring in new collaborators with expertise in the required disciplines.

Areas in existing basin models which particularly need strengthening or development are shown in Table 3. They include: (1) better libraries of petrophysical properties, including realistic data and mixing functions for mixed lithologies; (2) better ways of predicting heat-flow histories from local geologic information and principles of basin dynamics; (3) routine integration with seismic stratigraphy in order to estimate lithologies of undrilled sections; (4) routine consideration of threephase fluid flow (although in my opinion an approximate approach is just as valid as an exact mathematical solution, given our uncertainties about hydrocarbon compositions); (5) improvements in kinetic descriptions of thermal indicators (as discussed above); (6) better description and quantification of expulsion from source rocks; and (7) lack of quantification of hydrocarbon loss during migration. In addition, data on the kinetics of hydrocarbon generation from a greater variety of kerogen types, and improved kinetics of oil cracking would be valuable.

Other items shown in Table 3 which are nonexistent in all or most basin models include (1) the ability to handle faulting in any general way; (2) the inability to predict tectonic fracturing or to allow any fluid flow through non-matrix permeability (except through user-defined macroscopic faults manually inserted on the cross section); and (3) error/uncertainty/sensitivity analysis.

Table 3: Areas of basin modeling where improvements or development are particularly needed

Libraries of petrophysical properties
Predicting paleoheat flow from geologic history
Integration with seismic-stratigraphic data and models
Three-phase fluid flow modeling
Kinetics of thermal indicators
Understanding and quantification of expulsion
Quantification of hydrocarbon loss during migration
"Personalized" kinetics of hydrocarbon generation and cracking
General model for faulting
Predicting tectonic fracturing and fracture permeability
Error/uncertainty/sensitivity analysis

Some indication of the importance of these various omissions can be gained from the following statements:

1. In the future, much frontier exploration, where basin modeling might be very much in demand and of great potential value, will be carried out in tectonically complex areas. Basin models that cannot handle faulting will be unsatisfactory.

2. Matrix permeabilities are often calculated from porosities, but there is generally an uncertainty of at least an order of magnitude in such permeabilities (e.g., Magara, 1978). Large errors in estimating matrix permeabilities may lead to large errors in reconstructing fluid-flow patterns, which in turn may affect maturation and migration.

3. Where tectonic fracturing exists, fracture permeabilities will probably be several orders of magnitude greater than matrix permeabilities, and may thus control flow patterns (e.g., Larson *et al.*, in press). Ignoring fracture permeability may lead to major errors in reconstructions of fluid-flow histories.

4. Estimating hydrocarbon loss is both difficult and important (e.g., England *et al.*, 1987; Waples, in press b). For example, the relative attractiveness of the two prospects analyzed by Mackenzie and Quigley (1988) could have been reversed simply by adjusting the amount of migration loss within the uncertainties proposed by the authors themselves.

5. In a recent study of the Haltenbanken area (offshore Norway), two different companies came to opposite conclusions about the recent

heat-flow history of the area (Jensen and Dore, in press; Vik and Hermanrud, in press). The difference in the heat-flow history could have influenced timing and amount of hydrocarbon generation. Existing conceptual models for heat flow and basin evolution were not able to resolve this problem, even in a relatively well explored area where the period in question was very recent.

Poor applications

Weaknesses in applications of basin models include (1) poor integration of geologic and geophysical data into what are fundamentally a geochemical models; (2) inadequate training of modelers; and (3) inability to model interactively.

Many potentially useful sources of data are currently not being utilized by most basin models. Of particular value would be petrophysical data obtained by mathematical inversion of seismic data and wireline logs. Data from logs could supplement lithologic data based on sample analysis, and thus could make certain that realistic values of petrophysical parameters were being attached to each lithology. Data from seismic sections could help trace lithologic changes across areas lacking in well control. The importance of inserting good petrophysical data into the basin model can hardly be overemphasized.

As maturity modeling has become widely known and as commercial software has become more user friendly, maturity modeling has increasingly come to be seen as something that any geologist can do. However, although good geologists can teach themselves to do good maturity modeling (see Waples *et al.*, 1992a, b), formal training is highly advantageous. Basin modeling, which is much more complex than maturity modeling, requires even more training, but few companies are currently worrying about training for basin modeling.

Training in a discipline as complex as basin modeling is neither a one-day nor a one-step affair. Learning the necessary keystrokes is only the beginning of a good training program. Thorough indoctrination with a philosophy of modeling, complete familiarization with optimization procedures (see below), training in sensitivity analysis, familiarization with appropriate exploration applications, and extensive periods of practice should follow. The initial training required to allow someone to carry out modeling takes a few weeks, but full "licensing" of a geologist to execute basin-modeling studies independently could require a year or more of experience.

"Optimization" represents the search for combinations of input data (e.g., heat flow, amount of erosion, thermal conductivity) that will yield predicted output values in agreement with measured data (e.g., present-day temperatures, Ro values). Optimization must be carried out before hydrocarbon generation is modeled in order to ensure that input data are realistic and consistent (see Waples, in press a).

There are two major limitations to the effectiveness of optimization: personal skills and computer software (see next section). Personal skills can be enhanced by training. The modeler must first understand that the input data used in optimization should only be varied within geologically reasonable limits. Thus for all input parameters the modeler should recognize both the global limits and the limits constrained by local geologic history. Each input parameter must then be varied regionally in a geologically consistent and defensible manner. Therefore, prior to attempting to optimize the input data, the modeler must develop a coherent model for regional geologic history, based on data extracted from a number of geological, geophysical, and geochemical sources. Learning where to find such data, how to extract and interpret them, and how to build a coherent geologic model involves a large investment of time, and considerable skill.

The output data from any basin-modeling simulation will consist of precise numerical values for all parameters of interest. However, because of inadequacies of our scientific knowledge and equations, computer limitations, and uncertainties and errors in input data, the calculated values, however precise, cannot be expected to be completely accurate. In making exploration decisions, therefore, it is usually more useful to obtain a range of possible outcomes, each with a certain probability of occurrence (Fig. 2). This range of possible outcomes is generated using a range of input values designed to incorporate errors and uncertainty. Such methods are called "probabilistic," of which Monte Carlo simulations are the best known.

The goal of using probabilistic models is to help us perform sensitivity analysis, in which we investigate how much the final answer is affected if we vary each input parameter separately within our uncertainty limits for that parameter (e.g., Irwin *et al.*, in press). Training should provide a general understanding of the sensitivity of output values to changes in input parameters such as heat flow, thermal conductivities, and amounts of erosion; but it should also teach the user how to perform sensitivity analysis quickly and efficiently for the particular case being modeled. The ultimate objective of sensitivity analysis must be clearly understood by the modeler: to determine which of our uncertainties could lead to different exploration decisions.

Limitations in computer codes

Weaknesses in computer systems include (1) input-output systems that are not properly designed to take advantage of a geologist's strengths and ways of thinking, nor to facilitate data entry and manipulation; (2) simulation times that are too long to permit truly interactive modeling; and (3) lack of ability of the computer to aid in the optimization process. User interfaces must be designed by persons who are experts in all of the following areas: computer graphics, data bases, and user interfaces; exploration geology, geochemistry, and geophysics; and applications of basin modeling to exploration problems. In

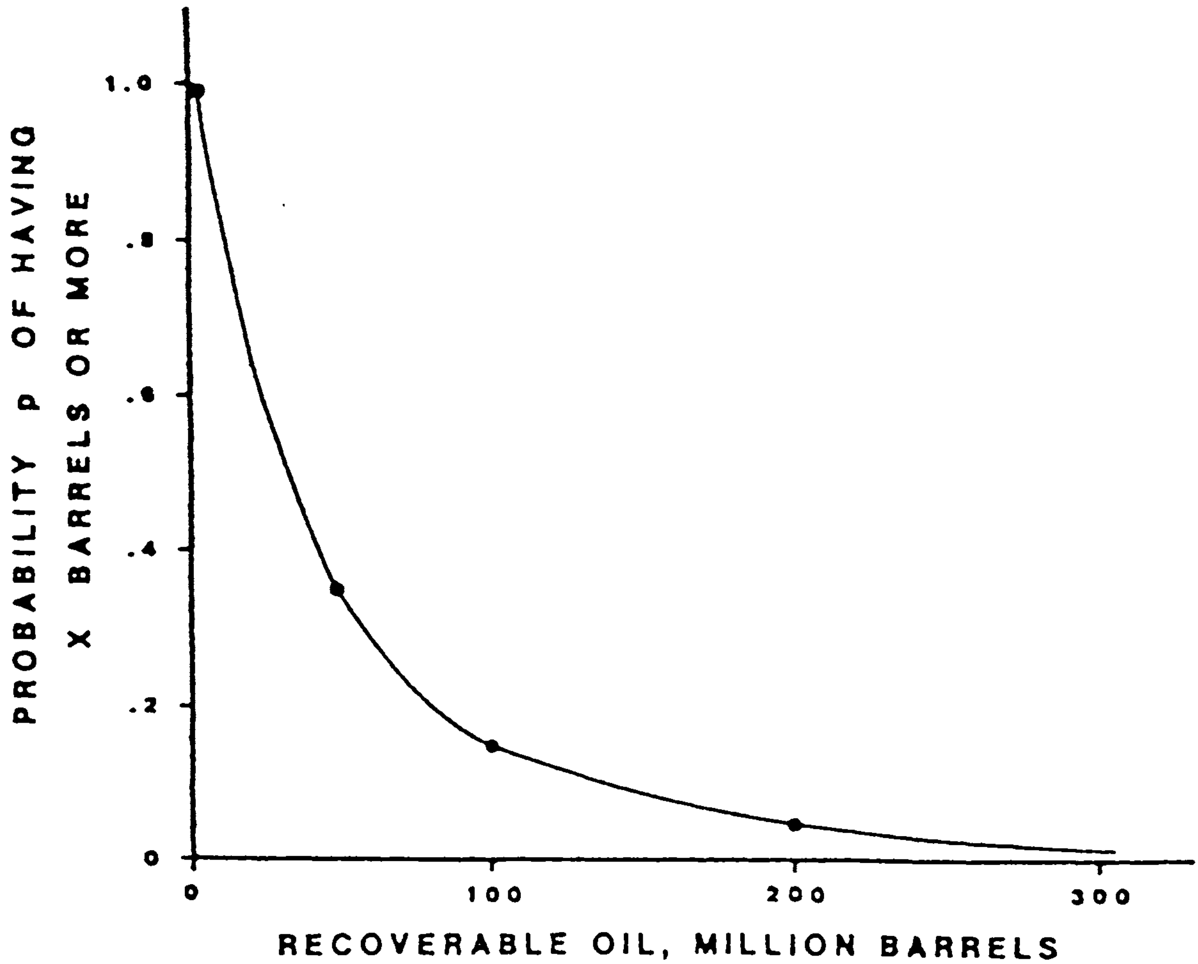

Figure 2: Example of output data from basin modeling calculated and presented in a probabilistic format. Vertical axis represents probability (0 is impossible, 1 is certain) that the recoverable oil will exceed the number on the horizontal axis. From Waples, 1984; reprinted with permission of the Rocky Mountain Association of Geologists.

rare cases a single person may embody those characteristics, but in most companies construction of such an interface will have to be a team effort, with all contributions regarded as equally important. Up to now the correct balance of expertise has seldom been achieved, and as a consequence user interfaces are not fully adequate. One obvious way in which well-designed interfaces could help would be in utilizing digitized forms of data routinely available to geologists (maps, cross sections, seismic sections, logs, etc.). Less obvious but potentially equally important would be more-subtle aspects, such as making it easy to enter and edit data for multiple locations, and to make global changes in a given variable.

Long simulation times can greatly decrease the interactive nature of the basin-modeling software, and thus decrease the convenience and quality of optimization, the amount of learning that occurs during modeling, and the quality of the final results of modeling. Optimization for 2-D or 3-D basin-modeling simulations is probably best carried out at individual points using l-D simulations. The advantage is that l-D modeling is much faster; the minor disadvantage is that phenomena like fluid flow cannot be adequately modeled in one dimension. However, any errors introduced during l-D optimization can be removed in a final optimization carried out in 2-D.

Unfortunately, optimization is a very difficult and tedious process if done manually, since a number of interdependent variables are manipulated simultaneously to find the optimal combination. In principle, computers should be ideally suited to performing optimization by following a series of rules, but little such development has occurred. The only computerization of the optimization process has been directed toward elucidating paleoheat flow by mathematically inverting a variety of thermal indicators (e.g., Lerche, 1988a, b). The main weakness with this approach is that it assumes other geological input data are correct, and that all uncertainty therefore rests in paleoheat flow. Consequently, as designed it cannot form the foundation of a complete optimization system, where all input variables are assumed to be imperfectly known.

The future

Despite the widespread attention being paid to development of basin models, and the interesting results that have been generated from modeling studies (e.g., Ungerer *et al.*, 1990; Dore *et al.*, in press), the future of basin modeling is far from certain. As mentioned previously, there is some justification for resistance to basin modeling, since early models have not been adequately attuned to the needs of exploration. If the ideas and needs of geologists and geophysicists can be integrated into future basin models, and if ways are found to allow sensitivity analysis to become a routine part of modeling, then basin models will have a bright future.

However, this bright potential will only be fulfilled if modelers are adequately trained to carry out modeling correctly. A fundamental decision remains to be made within each company interested in basin modeling. Will basin models become part of every geologist's workstation, or will modeling remain the province of a group of specialists? The best answer to this question may vary from company to company, depending upon its structure and the amount of training it is willing to provide to each geologist. Regardless of which path is chosen, however, it is imperative that all users of basin models be adequately trained, or else work with someone who is. Attention to this seemingly minor detail may prove to be the most important single item in developing a good basin-modeling system, since most experts agree that the ability of the modeler is more important than the details of the model.

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