Quantitative basin modeling: present state and future developments towards predictability

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ABSTRACT

A critique review of the state of quantitative basin modeling is presented. Over the last 15 years, a number of models are proposed to advance our understanding of basin evolution. However, as of present, most basin models are two dimensional (2-D) and subject to significant simplifications such as depth- or effective stress-dependent porosity, no stress calculations, isotropic fracture permeability, etc. In this paper, promising areas for future development are identified. The use of extensive data sets to calibrate basin models requires a comprehensive reaction, transport, mechanical (RTM) model in order to generate the synthetic response. An automated approach to integrate comprehensive basin modeling and seismic, well-log and other type of data is suggested. The approach takes advantage of comprehensive RTM basin modeling to complete an algorithm based on information theory that places basin modeling on a rigorous foundation. Incompleteness in a model can self-consistently be compensated for by an increase in the amount of observed data used. The method can be used to calibrate the transport, mechanical, or other laws underlying the model. As the procedure is fully automated, the predictions can be continuously updated as new observed data become available. Finally, the procedure makes it possible to augment the model itself as new processes are added in a way that is dictated by the available data. In summary, the automated data/model integration places basin simulation in a novel context of informatics that allows for data to be used to minimize and assess risk in the prediction of reservoir location and characteristics.

Key words: basin modeling, fluid flow, rheology

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THE NEW BASIN MODELING

Basin modeling, like any attempt to obtain quantitative predictions of a complex system, must be sufficiently comprehensive and, because of the great uncertainties involved, should be formulated in terms of probability theory. Here, we attempt to delineate steps that can be taken to achieve this goal and identify the benefits and pitfalls involved.

For the petroleum industry, a basin model is a set of rules (guided by laws underlying a set of physical and chemical processes) and computational techniques for predicting the location and characteristics of reservoirs. Thus, a model of a basin from this perspective is not just a sedimentologic history recreation software. It is not a maturation computation or a multiphase flow solver. It is not a rock deformation or heat transfer model. It is all this and more. And, in reality, it is also a methodology, either built into a software package or carried out by hand, to integrate all these physical and chemical processes with available geologic data.

Figure 1 suggests a set of reaction, transport, mechanical (RTM) processes that operate in a sedimentary basin. These processes are so strongly coupled that to leave out any of them is to risk failing to obtain reliable predictions of reservoir location and characteristics. For example, fracturing affects fluid flow, which changes pore fluid pressure and thereby fracturing, completing one of the many feedback loops underlying basin dynamics. Thus, while basin modeling apparently means many things to many people, we suggest that predictive basin models should be of the fully coupled, comprehensive RTM type.

The advantage of comprehensive RTM basin modeling is not only its potential for reliable predictions, but also its ability to predict a fuller suite of the parameters needed to characterize and evaluate a reservoir. They include the pressure

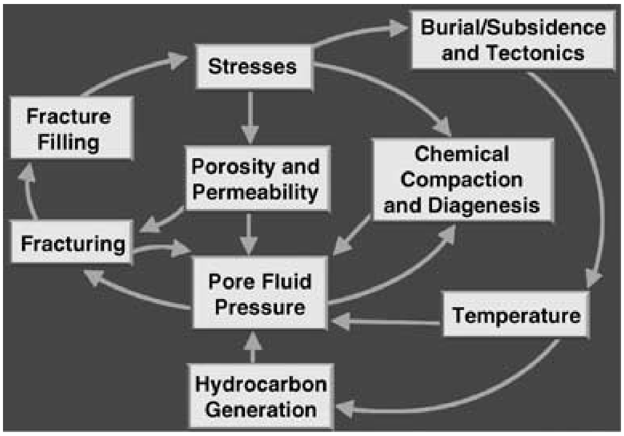

Fig. 1. Complex network of coupled processes underlying the dynamics of a sedimentary basin.

and composition of the various pore fluid phases, the shape, size, packing, and abundance of the minerals, fracture network statistics, and *in situ* stress. These rock and fluid parameters allow one to estimate reserves in place and the flow and mechanical properties of a reservoir needed to assess and optimize producibility.

We review a set of basin models and assessment of the subset of processes they account for in Table 1. As the models are often under active development, and as the actual processes being accounted for are not always made explicit in the literature, Table 1 is only meant to be suggestive of the state of the art, rather than to be complete.

The complexity of basin models is not the only challenge we must face. The volume of basin data, obtained at great expense, presents both a technical and economic challenge to the industry. What is needed is an automated procedure to derive value from these databases often available on a field or basin. From our research, we suggest that automated analysis can be achieved through model-automated informatics (MAI). By definition, informatics is the science of deriving conclusions or otherwise deriving information from a vast and complex database. In this article, we suggest that this can be achieved with the use of comprehensive basin model to analyze available data using information theory. Before presenting the details of the MAI strategy, we summarize the present state of basin modeling and the improvements that will be needed to integrate basin modeling with information theory to make it an economically viable exploration and field development technology.

Table 1 An incomplete but representative list of basin models.

Studies	Basin models
Ungerer *et al.* (1990)	2-D, ϕE, H, IIπ, SF, PG
Forbes *et al.* (1992)	2-D, ϕE, H, IIπ, PG
Person & Garven (1992)	2-D, ϕE, H, Iπ, PG
Maubeuge & Lerche (1993)	1-D, ϕE, H, Iπ, PG
Maubeuge & Lerche (1994)	2-D, ϕE, H, Iπ, PG
Bour & Lerche (1994)	2-D, ϕE, H, Iπ
Bredehoeft *et al.* (1994)	2-D, ϕD, Iπ, PG, SF
Wieck *et al.* (1995)	2-D, ϕE, H, Iπ
Person *et al.* (1995)	1-D, ϕD, H, Iπ, *PG*
Luo & Vasseur (1995)	2-D, ϕE, H, I
Yu & Lerche (1995)	2-D, ϕE, IIπ, PG
Roberts & Nunn (1995)	1-D, ϕE, H, Iπ, SF
Burrus *et al.* (1996)	2-D, ϕD, H, IIπ, PG
Luo & Vasseur (1996)	2-D, ϕE, IIπ, PG
Schneider *et al.* (1996)	1-D, IS with elasticity and viscosity, Iπ
Mello & Karner (1996)	1-D, ϕE, H, Iπ, SF
Luo *et al.* (1998)	2-D, elastoplastic rheology (cam-clay model), Iπ
Gordon & Flemings (1998)	1-D, ϕE, Iπ
Wang & Xie (1998)	1-D, ϕE, H, Iπ, SF
McPherson & Garven (1999)	2-D, ϕE/poroelasticity, H, Iπ
Schegg *et al.* (1999)	2-D, ϕE, H, IIπ, PG, SF
Lee & Williams (2000)	2-D, ϕE, H, Iπ, PG
Suetnova & Vasseur (2000)	1-D, IS with elasticity and viscosity
Payne *et al.* (2000)	1-D, IS with elasticity, viscosity, and fracturing, IIπ, SND, PG
Tuncay *et al.* (2000a,b)	3-D, IS with elasticity, viscosity, and fracturing, IIπ, 3-D SND, PG
Tuncay & Ortoleva (2001)	2-D, IS with elasticity, viscosity, and fracturing, IIπ, 3-D SND, PG
McPherson & Bredehoeft (2001)	3-D, ϕE, H, IIπ, PG
Stover *et al.* (2001)	2-D, ϕE, IIπ, H, PG

A list of earlier basin models was presented by Person *et al.* (1996). Representative list of basin models. Symbols indicate the following: H, heat flow; Iπ, single phase flow; IIπ, two-phase flow; ϕD, porosity–depth relationship; ϕE, porosity–effective stress relationship; SF , simple fracture model; PG, petroleum generation; IS, incremental stress rheology; and SND, statistical fracture network dynamics.

THE NEED FOR COMPREHENSIVE 3-D RTM BASIN MODELING

Overview

Nonlinearity and coupling are other reasons for constructing a comprehensive basin model. The modern theory of nonlinear dynamical systems has revealed their great potential for supporting a host of phenomena that arise autonomously, i.e. without their imposition by an external template. Nonlinear systems can, for example, oscillate periodically or chaotically in time and may organize spatially in regular patterns (see Nicolis & Nicolis 1987; Ortoleva *et al.* 1987a,b, 1990; Turcotte 1992; Ortoleva 1994a).

A necessary condition for autonomous spatio-temporal organization is met when the system is maintained sufficiently far from equilibrium (Nicolis & Prigogine 1977). The potential importance of nonlinear dynamics in geologic systems has been the subject of several conferences (Nicolis & Nicolis 1987; Ortoleva *et al.* 1990) and has been investigated extensively in the context of geochemistry (Ortoleva 1994a). For the sedimentary basin, it has been pointed out (Ortoleva 1994a,b; Tuncay *et al.* 2000a) that nonlinear dynamics can play an important role at a wide range of spatial scales. This potentially autonomous behavior suggests that many patterns of mineralization, petroleum reservoirs, fault motion, and other phenomena cannot be understood as direct consequences of related patterns of sedimentology, volcanism, or tectonism, i.e. cannot be attributed to an external template. Because of the large network of processes underlying basin dynamics, as well as the nonlinearity of the conservation equations, a computational modeling approach is likely the only way to delineate nonlinear basin phenomena and the range of conditions (overall tectonics, sedimentation history, etc.).

Far-from-equilibrium conditions, necessary for the operation of autonomous spatio-temporal patterning, can be obtained in a sedimentary basin. The basin is sustained out of equilibrium by the fluxes and forces applied at its boundary. Input of sediment presents the basin with minerals and fluid chemical species, which, after burial, are out of equilibrium at the local pressure and temperature or other conditions. Changes in tectonic forces, heat flux, or influxed magmatic or meteoric fluids can also cause all or part of the basin to be driven out of equilibrium. Other factors are the effect of overburden on compaction and buoyancy-driven flow (oil, gas, or hot aqueous liquid). These factors that drive the basin out of equilibrium are directly or indirectly imposed at the basin boundaries. Thus, as suggested in Fig. 2, the conditions inducing change within a basin may be expressed in terms of the boundary conditions imposed on the solution of the conservation equations. Rapid burial, large geothermal gradients, and large amounts of chemically unstable kerogen are examples of factors favoring an increase in the likelihood

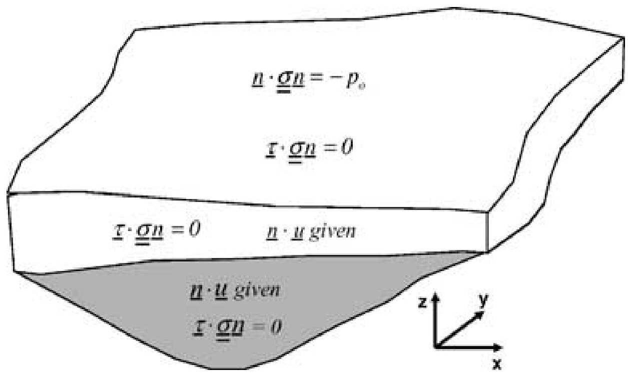

Fig. 2. Boundary conditions for stress ($\underline{\underline{\sigma}}$) shown here as well as those for heat and mass flow influence basin model predictions but are subject to great uncertainty. Conditions at boundary of basin simulation domain allow for imposition of ocean bottom normal pressure P_o and no shear at the top ($\underline{\tau}$ being a unit tangent vector and $\underline{n}$, an outward pointing unit normal vector with respect to the basin boundary). At the bottom, the tectonic history fixes the evolution of the deformation velocity $\underline{u}$ using slip conditions as on the sides (lightly shaded). The normal velocity $\underline{n}\cdot\underline{u}$ is imposed by the prescribed history of upheaval/subsidence and compression/extension.

of autonomous basin behavior. Comprehensive, three-dimensional (3-D), fully coupled models are designed to capture this richness in autonomous basin behavior.

Although 1-D and 2-D studies give insights into the dynamics of basin evolution, a 3-D basin simulator is necessary to take all geometric effects into account. This becomes extremely important when fracturing is mainly because of flexure and the direction of tectonic compression/extension is changing over the basin's history. Fracture networks provide a pathway for fluid flow and, especially in a layered medium, fluids can move laterally. This can only be taken into account by a 3-D basin simulator with a stress/deformation solver that can capture the nonplanar layers (notably domes) and the strong variations in rheology from layer to layer. The fundamentally 3-D nature of these systems is further enhanced as preferred fracture orientation induces an anisotropic permeability tensor that can strongly influence the direction of fluid flow. Table 1 summarizes the spatial dimensionality and RTM processes of a number of basin models. In the next subsections, we discuss two important basin phenomena to illustrate the need for a comprehensive 3-D modeling approach.

Compartmentation

A compartment is a zone of fluid trapped within an envelope of low permeability rock. Compartmentation is viewed as a nonlinear phenomenon arising from the dynamics of the crustal fluid-rock system (Ortoleva 1994a,b, 1998; Ortoleva *et al.* 1995). This view leads to insights into the origins of compartments and the complex dynamics of the exchange of fluids with their surroundings.

Compartments are found in sedimentary basins worldwide. Such domains of rock, typically with abnormal fluid pressures, have been recognized for many years in the petroleum industry (Dickey & Cox 1977; Powley 1990; Al-Shaieb *et al.* 1994; Bradley & Powley 1994; Ortoleva 1994a,b, 1998; Ortoleva *et al.* 1995). Powley (1980) has given evidence that sedimentary basins are typically divided into a boxwork of compartments, each of which are bounded on top, bottom, and sides by seals. Diagenetic, hydrologic, and mechanical processes underlying the development and dynamics of compartments are outlined by Ortoleva (1994a,b, 1998) and Ortoleva *et al.* (1995).

A key element of compartmentation appears to be the existence and inter-relationships between phenomena on a broad range of length scales. What is, in fact, most interesting and important is that the phenomena on these wide range of scales may strongly couple to reinforce each other in many ways. Let us define these scales, and then note some of their inter-relationships.

Microscale phenomena are defined here to be those that take place on a length scale of the order of a single or perhaps few grain diameters. Most notable among these phenomena are grain growth/dissolution/nucleation reactions, grain coating, plastic grain deformation, microfracturing/breakage, and rearrangement. These processes underlie compaction and porosity/permeability occlusion or enhancement.

Mesoscopic phenomena take place on the 10-grain diameter to meter scale. A key aspect of mesoscopic phenomena is that they involve a statistically significant number of grains so that they might be described in terms of the spatial distribution of the local texture. Texture is taken to mean the average grain volume, shape and orientation of the various minerals present but could be more detailed – that is, be described in terms of the probability distributions for the aforementioned quantities. Examples of mesoscopic phenomena are stylolites, banded compaction/cementation alternations, differentiated or enhanced marl/limestone alternations, and banded carbonate cements in sandstones (Dewers & Ortoleva 1990a, 1994a; Ortoleva 1994a,b; Qin & Ortoleva 1994).

Macroscopic phenomena are exemplified by intra-lithologic unit compartments or those encompassing several lithologic units. They exist on the 10-m to 10-km scale, laterally. The largest (basin) scale is the megascopic scale. A megacompartment may have a complex, nested interior structure of smaller scale compartments.

Phenomena on all these scales are intimately related. Mesoscopic processes involve the spatial distribution of microscopic variables. In turn, the conditions promoting or repressing the processes (stress or fluid pressure, for example) are affected by macro- and megascopic phenomena. Mesoscopic phenomena can create seals and hence play a key role in defining the boundaries of a compartment on the macro- or megascopic scale. In summary, phenomena on one scale affect and are affected by phenomena on one or more other scales – compartmentation involves a complex network of cross-coupled processes operating on a hierarchy of scales.

Salt tectonics

While salt tectonic phenomena have long been recognized as a key process in basin evolution and, in particular, in the context of petroleum reservoir location and characteristics, most studies have not addressed the complexities caused by the interplay of salt deformation with other RTM processes.

Salt tectonics features are the consequences of a symmetry breaking of the idealized planar state of a salt layer over- and under-lain by other horizontal sediments. Small disturbances in the translational invariance of the system in the horizontal directions can be amplified by the RTM processes into wave, diapir, and more complex features. The controversy as to the physical laws underlying salt tectonics, and hence, in our view, the aforementioned self-organization, still has not been completely resolved (Koen 1993; Taylor 1995; Tuncay & Ortoleva 2001). We believe that this is because, while one can rather easily conjecture a variety of mechanisms, it is likely a quantitative question as to which ones dominate in a given geologic context. Experience gained over the past three decades in nonlinear dynamical systems shows that they often behave in rather unexpected ways. A solution to this dilemma is to study salt tectonics using a comprehensive, 3-D multi-process simulator. In such an approach, one may test the relative importance of the various factors and evaluate the degree to which they reinforce or inhibit one another.

Although there is a vast number of observations of salt structures (Seni & Jackson 1984; Jackson & Talbot 1986; Cobbold 1993), there are only a few attempts to numerically simulate them. Most salt simulators are 2-D, and both salt and sediment are treated as bulk materials, i.e. fluid flow through the pores and its influence on effective stress are ignored. None of these models account for the evolving rheology of the sediments because of diagenesis and mechanical processes, petroleum generation, and the changing thermal regime. Therefore, most salt tectonics simulators do not have the sufficient comprehensiveness that can assist salt-related exploration.

Daudre & Cloetingh (1994) presented a 2-D analysis based on Stokes flow. In this approach, both sediment and salt are treated as nonlinear viscous fluids. A Drucker–Prager criterion is adopted to model the inception of brittle deformation. The density of sediment was calculated based on a pressure-dependent porosity. An updated Lagrangian formulation was used to simulate large deformations. They showed that extension combined with salt rheology favors salt diapirism. Van Keken *et al.* (1993) obtained the effective rock salt viscosity by adding dislocation creep and pressure solution creep. The effective salt viscosity was allowed to depend on temperature, strain rate, and grain size. Pressure solution dominated the salt motion. Sediment density was taken to be a function of depth. With these assumptions, they performed a sensitivity analysis for the effect of overlying sediment viscosity. Their results showed that the sediment viscosity/salt viscosity ratio is an important factor in determining salt motion and geometry. Another 2-D model was developed by Mazariegos *et al.* (1996) based on Stokes flow. They used two different salt rheologies; a dislocation-creep power law and a fluid-assisted creep law. The functional form of the salt rheology depended on grain size. Although they used a rather complex rheology for salt, sediment viscosity was taken to be constant. They showed that their fluid-assisted creep law results in faster salt motion. They concluded that a better understanding of salt diapirism requires an accurate characterization of surrounding rock rheology. A 2-D study was presented by Schultz-Ela *et al.* (1994) who used the commercial program GEOSIM-2D for their numerical modeling. Salt was treated as a visco-elastic material, whereas sediment was modeled with an elastoplastic rheology. Plastic yield was determined with a Drucker–Prager criterion.

In all of these studies, the results were limited to 2-D. However, the most crucial difficulty is that they are limited to the deformation of bulk media. In other words, they do not employ the theory of composite porous media. In composite environments, the velocity, stress, and other descriptive variables of solid and fluid phases show very different time history and spatial distributions. For example, the velocity and stress tensor of solid and fluid phases are very distinct. Therefore, although approximation of such a complicated composite medium by an equivalent bulk medium may give some information, it cannot have the predictive power of a composite model.

Recently, Tuncay & Ortoleva (2001) presented a 3-D model that accounts for poroelasticity, nonlinear temperature-dependent viscosity, 3-D fracture network dynamics, and multiphase flow with petroleum generation. They also studied the role of the coupling between the spatial distribution of sediment input rate and diapir growth, and demonstrated the genesis of subsalt compartments, coordinated migration of petroleum and fracture network dynamics, and salt morphology.

IMPORTANT PHYSICAL AND CHEMICAL PROCESSES

Stress and deformation

Reconstructing the stress and deformation history of a sedimentary basin is a challenging and important problem in the geosciences with a variety of applications. These include petroleum exploration, reserve assessment and production, and earthquake hazard reduction. Progress in this field has been hampered by the absence of an integrated mechanical modeling approach set within the wider context of the coupled RTM dynamics of a basin.

The strongly coupled nature of basin deformation may be understood in terms of the feedbacks underlying crustal dynamics. For example, pore fluid pressure affects stress, stress changes can lead to fracturing, and fracturing can affect pore fluid pressure. Similarly, stress can affect mineral solubility, the latter can cause mineral dissolution which, in turn, can affect rock rheology and hence stress. Clearly, basin deformation requires an accounting of the coupling among the many RTM processes. Therefore, modeling sedimentary basin dynamics requires a fully coupled approach.

The goal of the modeling is to calculate the evolution of the distribution within a basin of the set of descriptive variables characterizing its internal state:

- rock texture and mineralogy;
- fluid properties;
- temperature;
- rock deformation;
- fracture network characteristics; and
- stress.

These properties respond over geologic time to their interactions among each other and via the influence of the basin's surroundings. The interaction with the surroundings provides the boundary conditions to which the equations of mass, energy, and momentum conservation must be subjected to arrive at the evolution of the basin. In this way, basin analysis becomes the delineation of the RTM basin dynamical system and its response to the constraints imposed at the boundaries. As the laws for the basin RTM processes are nonlinear in the descriptive variables, one expects this response to be extremely rich (Dewers & Ortoleva 1994a; Ortoleva 1994a,b, 1998).

An important limiting assumption made in most basin models is that there exists a simple dependence of porosity on effective stress (Ungerer *et al.* 1990; Forbes *et al.* 1992; Person & Garven 1992; Maubeuge & Lerche 1993, 1994; Bour & Lerche 1994; Luo & Vasseur 1995, 1996; Roberts & Nunn 1995; Wieck *et al.* 1995; Yu & Lerche 1995; Yu *et al.* 1995; Mello & Karner 1996; Schneider *et al.* 1996; Gordon & Flemings 1998; Wang & Xie 1998; McPherson & Garven 1999; Schegg *et al.* 1999; Lee & Williams 2000; Polyansky & Poort 2000; McPherson & Bredehoeft 2001) or depth (Bredehoeft *et al.* 1994; Person *et al.* 1995; Burrus *et al.* 1996). Different compaction parameters are used for shales and sandstones regardless of their mineral composition, and grain size distribution. Although these approximations allow fast computations, they lack the effects of compressional/extensional regimes, brittle deformation (such as fracturing), heat flux, and rock texture on porosity evolution. Such expressions might result in limited success for a well-studied basin with a large set of data. However, their applicability to new prospects is doubtful as the parameters calibrated for a mature basin include the unique geologic boundary histories (overall tectonics, heat and fluid flux at the boundaries) that influenced it. In summary, these models do not account for the unique history of pressure, stress, and temperature to which the medium was subjected. The conservation laws are universal; it is the differences in the history of the evolving boundary conditions that give a basin its individual character.

The difficulty in modeling deformation in porous media stems from the many deformation processes that operate over long time scales. The integration of these processes can be achieved using an incremental stress approach. In analogy with the classic theory of chemical kinetics, the total rate of strain $\dot{\underline{\underline{\varepsilon}}}$ is written as a sum of terms

$$\dot{\underline{\underline{\varepsilon}}} = \sum_{j=1}^{N} \dot{\underline{\underline{\varepsilon}}}^{(j)}. \tag{1}$$

The list of such processes includes:

- poroelasticity;
- continuous, irreversible rock deformation;
- fracturing; and
- pressure solution.

The outstanding contributions of incremental stress theory is that the total rate of strain is expressible as a linear combination of rate of strains from different processes due to the fact that it represents a relation among infinitesimal changes. The individual rate of strain terms on the right-hand side of equation 1 depend on the full suite of rock textural and fluid properties as well as the macroscopic stress. it is through this dependence and the coevolution of rock deformation and of these variables that the full coupling of all processes is accounted for in a model. As the rates $\dot{\underline{\underline{\varepsilon}}}^{(j)}$ typically vary more strongly than linearly with these variables, the basin is a nonlinear dynamical system.

The poroelasticity term depends on the elasticity tensor of the medium, effective stress coefficient, total stress, and fluid pressure. The elasticity tensor depends on the instantaneous mineral composition, fracture statistics, grain sizes, temperature, and porosity. As these quantities (fracture statistics, temperature, etc.) evolve, the elasticity parameters change accordingly. The challenge is the calculation of the individual rates of strain for a multimineralic rock as it requires the homogenized response of the medium. For example, given the mineral elasticities, grain sizes, and porosity, the bulk and shear moduli, and effective stress coefficients of the (assumed) isotropic rocks can be computed using Berryman's composite medium theory (Berryman 1980, 1986, 1992).

A direct coupling of mechanics and chemistry arises through pressure solution. Grain dissolution at stressed grain–grain contacts induces compaction and, thereby, contributes to the total rate of strain. The rate of this pressure solution contribution, depends on the stress at grain–grain contacts and hence on the macroscopic stress, fluid pressure, and texture. However, it should also depend on the composition of the pore fluid. Pressure solution-derived rates of strain must be formulated through a relation between the rate of change of variables characterizing the texture and through a geometric relation between texture and macroscopic strain (Weyl 1959; Dewers & Ortoleva 1994b; Renard *et al.* 1999a,b).

Another effect that is usually disregarded is the volumetric strain caused by fracturing. As fractures open, the overall rock volume increases and fluid pressure decreases (because of flow and increase in pore volume). This reduces the rate of fracture growth. Therefore, fracturing is a self-limiting process.

Example boundary conditions that are needed to complete the formulation of the rheologic problem are illustrated in Fig. 2. These conditions enforce the lateral compression/extension and subsidence/upheaval imposed by the larger scale tectonics. The interaction of the top of the sediment pile with the overlying fluids (atmosphere or sea bottom) is accounted for by the value of normal stress and the (assumed) absence of tangential shear. A no-vertical-shear lateral boundary condition allows for natural compaction at the sides of the basin.

There are a few basin-modeling studies that consider incremental stress rheology. Among them, one can note Dewers & Ortoleva (1994a; 1-D incremental stress rheology accounting for poroelasticity and pressure solution with single-phase flow), Suetnova & Vasseur (2000; 1-D visco-elastic rheology with single phase flow), Schneider *et al.* (1996; 1-D visco-elastic rheology with single phase flow), Luo *et al.* (1998; 2-D elastoplastic rock behavior with single phase flow), Tuncay *et al.* (2000a,b), and Tuncay & Ortoleva (2001; 3-D incremental stress rheology accounting for poroelasticity, nonlinear viscosity, and fracturing with multiphase flow).

Multiphase flow

Multiphase flow in porous media is of interest in various areas of science. Significant amount of effort has been spent on different aspects and applications of multiphase flow in porous media such as contamination of groundwater aquifers, reservoir modeling, and basin evolution. The main difference between these applications is the magnitude of the time scale. The engineering time scale contamination or recovery operations can vary from days to months, whereas the time scale for basin evolution is in the order of millions of years. Therefore, the numerical approach followed for large time scale problems must allow large time steps, and must be accurate enough to capture the nonlinear dynamics of the problem. Furthermore, the dynamic nature of the basin evolution because of the time-dependent sedimentation, extension, subsidence, and erosion makes the problem computationally very challenging. Another complexity is the range of material properties such as permeability in basins. The permeability range may be as large as 10 orders of magnitude. This requires the use of a mesh that is locally adapted to the material discontinuities.

Numerical models for multiphase flow in porous media have been presented by various researchers based on finite difference and finite element methods. These models focused on surface spills and subsurface leakage of hydrocarbons from pipes and storage tanks (Kaluarachchi & Parker 1989; Celia & Binning 1992; Sleep & Sykes 1993a,b; Huyakorn *et al.* 1994; Panday *et al.* 1994, 1995; White 1995; Hadad *et al.* 1996) and reservoir simulation (Young & Stephenson 1983; Watts 1986; Quandalle & Sabathier 1989; Sukirman & Lewis 1993). In parallel with the advances in computer hardware, the simulators have started to employ implicit numerical techniques with applications to miscible multiphase flow problems. Newton–Raphson linearization appears to be the most popular technique in the solution of nonlinear algebraic equations, which makes the need for fast large-sparse-matrix solvers inevitable (Kipp *et al.* 1992; Peters 1992). A review of trends in numerical modeling of multiphase flow in porous media is given by Panday *et al.* (1995).

The potential role of petroleum in creating traps and preserving the porosity needed to house it has long been recognized in the petroleum industry (Wilson 1977; O'Brien & Lerche 1986). Multiphase flow models in basin simulators have mostly been limited to immiscible two-phase flow (Ungerer *et al.* 1990; Forbes *et al.* 1992; Burrus *et al.* 1996; Luo & Vasseur 1996; Tuncay & Ortoleva 2001) or miscible two-phase flow (Payne *et al.* 2000; Tuncay *et al.* 2000a). Yu & Lerche (1995), McPherson & Bredehoeft (2001), Wendebourg (2000) and Schegg *et al.* (1999) presented three-phase multiphase flow in the context of basin modeling. Modeling of multiphase flow in deforming porous media requires rock texture- and fluid composition-dependent relative permeability and capillary pressure curves. In the absence of experimental data, expressions provided by Brooks & Corey (1964) and Van Genuchten (1980) are the most commonly used ones (see Lenhard *et al.* 1989b for a comparison). Although empirical parameters are introduced to model the observed hysteresis in flow parameters (Parker & Lenhard 1987; Lenhard *et al.* 1989a), they have not apparently been applied to basin scale problems yet.

Petroleum generation

The thermal degradation of organic material leads to the creation of components (methane and other C- and H-rich molecules), which add to the pore-filling fluid phases. For organic-rich lithologies [coal or high total organic carbon (TOC) shale], organic reactions can cause compaction or shrinkage. Reaction-induced matrix shrinkage causes cleating in coals and may lead to similar effects in organic-rich shales. Models of kerogen breakdown and other organic reactions are required to study the time course of the generation of petroleum. A number of such models are available (Tissot *et al.* 1987; Espitalie *et al.* 1988; Braun & Burnham 1990; Hunt *et al.* 1991; Pepper & Corvi 1995). However, these models are highly schematic and are calibrated to the organic material from various basins but not to the detailed network of reaction processes among specifically identified molecules or sites on macromolecules. Thus, it seems that results from one type of material, basin, or context cannot be easily generalized to others.

A fundamental component of most existing basin models is petroleum generation (Ungerer *et al.* 1990; Forbes *et al.* 1992; Person & Garven 1992; Bredehoeft *et al.* 1994; Person *et al.* 1995; Yu & Lerche 1995; Burrus *et al.* 1996; Luo & Vasseur 1996; Mello & Karner 1996; Forster *et al.* 1998; Schegg *et al.* 1999; Lee & Williams 2000; Payne *et al.* 2000; Wendebourg 2000; Tuncay *et al.* 2000a; McPherson & Bredehoeft 2001; Tuncay & Ortoleva 2001; Payne & Ortoleva 2002a,b). The generated petroleum is used as a lumped source term in the mass balance equation for the oil or gas phase, i.e. the detailed composition of products is not taken into consideration.

To overcome the limitations of relatively simple petroleum generation models, the following must be addressed:

- More complex equations of state.
- Detailed mechanisms allow greater number of activation energies and thus greater predictability of the relations between thermal histories and gas composition.
- Temperature/overpressure relationship.
- Coupling to organic reactions.

Heat flow

It is a common practice to assume that the solid phase is in thermal equilibrium with the fluid phase. Classical advective–dispersive heat transfer equation is used to model heat flow (Ungerer *et al.* 1990; Forbes *et al.* 1992; Person & Garven 1992; Person *et al.* 1995; Roberts & Nunn 1995; Wieck *et al.* 1995; Mello & Karner 1996; Forster *et al.* 1998; Wang & Xie 1998; McPherson & Garven 1999; Polyansky & Poort 2000; McPherson & Bredehoeft 2001). A specified temperature is imposed at the interface between sediment pile and sea, and heat flux history is applied at the bottom of the sediment pile. The lateral boundaries are assumed to have zero heat flux. Some models have considered radiogenic heat production (Mello & Karner 1996; Forster *et al.* 1998).

As rheology is affected by temperature, and as deformation affects, the spatial distribution of thermal conductivity, heat transfer, and deformation problems must be solved simultaneously – an issue particularly important in salt tectonic regimes (Tuncay & Ortoleva 2001).

Fracture mechanics

Fractures play an important role in many geologic processes. They provide a mechanism of deformation and a pathway for fluid flow. The timing of fracture initiation and the scenario of their evolution over the history of a zone may significantly affect the rate and direction of fluid migration.

Because of its importance to both petroleum and geologic sciences, fracturing has been studied by many researchers (see Pollard & Aydin 1988; Lorenz *et al.* 1991 for reviews). Fractures in areas subjected to bending are usually explained by associated extensional stresses (Friedman 1976). The existence of fractures in near-horizontal layers has been attributed to unloading (Currie & Nwachukwu 1974; Engelder 1987), high fluid pressure (Pollard & Aydin 1988; Ortoleva 1998), and anisotropic stress influenced by nearby geologic structures (Currie & Nwachukwu 1974; Segall & Pollard 1983). Clearly, fracturing in near-horizontal or folded areas is because of a combination of the effects listed above. If the local fracture kinetics is well described by fracture growth/healing laws, a multiprocess deformation model coupled to fluid flow and fracturing can be used to quantify the relative importance of these effects.

It is well documented that fracturing strongly depends on lithology (Kulander *et al.* 1979; Segall & Pollard 1983; Hancock *et al.* 1984; Lorenz *et al.* 1991; Gross 1993; Fischer *et al.* 1995; Wu & Pollard 1995). Although fracturing can occur in almost any type of rock, they are more common in brittle rocks (Mallory 1977). Furthermore, fractures in a brittle lithology commonly discontinue at the interface of more ductile lithologies (Engelder & Geiser 1980). Another observation is that fracture spacing is strongly dependent on bed thickness and lithology (Harris *et al.* 1960; Nickelsen & Hough 1967; Gross 1993; Fischer *et al.* 1995; Wu & Pollard 1995). However, a simple correlation between fracturing and bed thickness does not seem feasible because of the many factors operating such as fluid pressure, state of stress, neighboring lithology properties, and tectonics.

Present-day flexure is often a poor indicator of fracturing. If the rate of flexure development was very slow, then there would be no fracturing. Also, flexure early in a sedimentary rock's evolution (i.e. when it is poorly lithified) or if sediment has inherent ductile behavior (as for organic-rich shales, rock salt or anhydrites) can occur without fracturing. Thus, prediction of present-day fracturing requires a model that allows for the continuous processes (notably ductile behavior or pressure solution) to compete with discontinuous deformation (faulting and fracturing) to arrive at the overall deformation.

Fracturing may introduce anisotropy to the evolving system. Fractures orient flows along their surface and also introduce directions of weakness in a deforming rock. Thus, fractures may guide the direction of high pressure fluids, which thereby changes the location of subsequent fracturing. Fracture-induced changes in rheologic parameters may affect the overall stress tensor, which, in turn, affects the orientation of subsequent fracturing.

In most basin models, it is assumed that rocks fracture when the fluid pressure exceeds a specified fraction of lithostatic (Ungerer *et al.* 1990; Maubeuge & Lerche 1993, 1994; Bredehoeft *et al.* 1994; Roberts & Nunn 1995; Luo & Vasseur 1996; Mello & Karner 1996; Schneider *et al.* 1996; Wang & Xie 1998). This assumption essentially eliminates the dependence of fracturing on lithologic properties, although it is well known that fracturing strongly depends on texture (Harris *et al.* 1960; Nickelsen & Hough 1967; Mallory 1977; Segall & Pollard 1983; Lorenz *et al.* 1991; Gross 1993; Fischer *et al.* 1995; Wu & Pollard 1995). Such a simplification also fails in predicting nonvertical fractures because of flexure.

In most of the existing basin evolution simulators, fracture permeability is assumed to be isotropic (Ungerer *et al.* 1990; Maubeuge & Lerche 1993, 1994; Bredehoeft *et al.* 1994; Roberts & Nunn 1995; Luo & Vasseur 1996; Mello & Karner 1996; Schneider *et al.* 1996; Wang & Xie 1998). This is apparently because of the lack of information in their models about the tensorial nature of the stress tensor and the resulting, evolving fracture network.

There is a vast amount of work on approximations for the permeability of fracture networks (for example, Oda 1986; Long & Billaux 1987; Odling 1992; Berkowitz 1995; Koudina *et al.* 1998). However, in these studies, a fracture network is generated either by an independent (decoupled) statistical, geometrical model or based on data.

To account for the above effects, forward quantitative basin models should include:

- fracture orientation reflecting the stress tensor;
- new fractures are added to the evolving network as the stress tensor changes because of tectonics or to fracture or diagenetic changes in rheology;
- the fracture network characteristics affect the tensorial fluid transport (e.g. permeability) and rock rheologic parameters;
- the construction of rose diagrams and other parameters that can be compared with observation; and
- an account of the mineralogy, texture, and statistical variations of properties (notably weak spots) that can affect fracturing and change over the geologic time scale.

Recently, Tuncay *et al.* (2000b) presented a dynamical model of fracture growth that is fully coupled to other crustal processes, deformation, and heat transfer. Thus, the oscillatory and other self-organization and nonlinear phenomena of crustal evolution can be captured (Ortoleva *et al.* 1987a,b; Maxwell & Ortoleva 1994; Dewers & Ortoleva 1994a; Ortoleva 1994a,b). The most notable of these is the cycle of fracturing → fluid flow → fluid pressure release → fracture healing (Ghaith *et al.* 1990; Chen *et al.* 1994; Dewers & Ortoleva 1994a; Ortoleva 1998). Modifications were made to the fracture length growth law that allows for fracture healing. In their model, each representative volume of rock is given a statistical distribution of fracture nuclei and associated tensile strength. This is a way to approximate the effect of rock heterogeneity and fracture interaction, and to predict the density of fractures and their dependence on the histories of stress, fluid pressure, and rock properties. A formalism is developed to account for the orientation of single or multiple fracture sets. The model is thereby able to describe conditions for developing a few large fractures or a swarm of smaller ones, depending on the rate of change of fluid pressure and stress. The change in the rock volume and anisotropic fracture permeability tensor are also obtained.

UNCERTAINTIES IN BASIN MODELS

Overview

Although basin models require a large number of phenomenologic parameters as well as geologic boundary conditions, only a few studies focused on the utilization of observed data to constrain the model (Lerche 1991; Maubeuge & Lerche 1993; Zhao & Lerche 1993; Yu *et al.* 1995; Tuncay & Ortoleva 2002). Yu *et al.* (1995) used observed porosity, permeability, fluid pressure, and layer thickness data to evaluate two parameters that appear in empirical porosity and permeability expressions. However, their study lacks the assessment of uncertainty associated with the predictions.

Uncertainties in the input data needed to run a basin model lead to uncertainties in the predictions. Furthermore, formulating this input data is an extremely labor-intensive and subjective process. We suggest that basin modeling is naturally placed within the context of probability theory as follows. Let $\rho[B]$ be the probability of the boundary tectonic scenario B. The objective is to construct $\rho[B]$ and thereby find the most probable B. Once the most probable B is determined, we can use it with the basin model to predict the likely location and characteristics of the reservoirs in a study area. As we have $\rho[B]$, we can also determine the uncertainties in any of the reservoir location and state parameters. With this, the basin-modeling effort should focus on the development of basin data collection procedures that reduce the uncertainties implied quantitatively by the form of the dependence of ρ on B.

As the objective is to decrease uncertainty, we wish to obtain sufficient information to limit the range in B over which ρ is nonnegligible. Information theory (Jaynes 1957) provides a general prescription for constructing $\rho[B]$ using the information we know about the system. This procedure is outlined in Information theory formulation. It is shown there that seismic, well-log, core, and other data can be used to constrain ρ if the basin model is sufficiently comprehensive that it predicts enough fluid and rock properties to construct synthetic seismic, well-log and other data. While the difference between the observed and synthetic data provides an error that can be minimized to calibrate a few model parameters, it cannot, given the sparseness of real data sets, give the most probable boundary tectonic scenario, nor can such an error minimization procedure yield a self-consistent assessment of risk. The procedure outlined in Information theory formulation enables one to surmount these difficulties.

A probabilistic basin-modeling approach can also provide a natural platform for the integration of expertise. These expertise constraints include limiting the spatial and temporal scale of phenomena (e.g. maximum known rate of overall basin deformation, basement heat flux, etc.). In the section under Information theory formulation, we show that this can conveniently be performed via the minimum relative entropy approach. As a model becomes more comprehensive or the number of expertise constraints are increased, less data are needed. If the above data/modeling integration can be automated, a basin model in effect becomes the centerpiece of a database mining algorithm as differential equations of physics and chemistry are simply algorithms for processing information. In this sense, this procedure is the essence of a quantitative geoinformatics methodology.

Phenomenologic parameters

Modeling a large number of RTM processes requires information on a rather large set of parameters that appear in the equations of mass, momentum, and energy conservation, and phenomenologic laws. Most of these parameters are subject to uncertainties.

Rock rheology

The bulk and shear elastic moduli of minerals are fairly well known. However, existing composite medium approximations are based on wave scattering for simple geometries. The effective viscosity of a multimineralic rock poses one of the most difficult homogenization problems. As experimental data in the range of temperatures of interest are very limited, parameters that appear in the phenomenologic expressions are subject to great uncertainty. Currently, most of the experimental studies in this area focus on the compaction. Even if the medium is isotropic, there is need for additional information on the irreversible distortional rock deformation.

Multiphase flow parameters

The relative permeability and capillary pressure relations evolve as rock texture and fluid composition change. Therefore, using present day relationships throughout the simulations is a very crude approximation. There is need for development of expressions that account for grain size distribution, porosity, fluid composition, and temperature. Calculation of matrix and fracture permeability tensors requires a sufficiently rich texture model that includes many variables to describe the medium. This aspect is briefly discussed in the section under Incorrect and/or incomplete models.

Geologic boundary conditions

For practical reasons, basin analysis is based on sparse and irregularly distributed data. Basin analysis involves reconstructing the spatial geometry of sedimentary bodies in three dimensions or reconstructing the detailed history of sediment input/erosion across the basin, and a number of commercial software focus on this aspect of basin modeling. Such information is invaluable in unraveling the history of the basin and for applications such as mineral and oil exploration, hydrocarbon reservoir simulation, and resource assessment.

To be effective, such a reconstruction must have a number of key attributes:

- automation so that new data can continuously be added for re-evaluation;
- automatic output of cross-sections and 3-D graphical representations;
- respect of general knowledge of sedimentary body geometry, sharpness of property changes across contacts, and smooth variations within a lithologic unit; and
- respect of irregularity of well location and depth/time interval of available mineralogic, age, and textural information.

Thus, an effective approach must transform sparse, irregularly distributed data into a basin-covering picture that respects notions of sedimentology and can be continuously and automatically updated.

Perhaps the most error-prone of basin model input data is the 'tectonic boundary scenario' B:

$$B = \text{time course of} \begin{cases} \text{uplift/subsidence} \\ \text{compression/extension/wrenching} \\ \text{basement heat and mass flux} \\ \text{sedimentation/erosion} \\ \text{climate/sea level} \end{cases} \quad (2)$$

This tectonic boundary scenario constitutes a continuous infinity of parameters (the value of these parameters over all the surface of the basin, for all times) that are traditionally determined in labor-intensive fashion and subject to individual bias.

Incorrect and/or incomplete models

Multiphase flow in fractured porous media

There is a vast amount of experimental data on relative permeabilities and capillary pressure relations (Brooks & Corey 1964; Lenhard & Parker 1987; Nordtvedt *et al.* 1997; Liu *et al.* 1998). In the absence of experimental data, expressions provided by Brooks & Corey (1964) and Van Genuchten (1980) are the most commonly used ones (see Lenhard *et al.* 1989b for a comparison). However, because of the sensitivity of parameters to rock texture, and fluid configuration and properties, and hysteresis in the relations, a unified model has not been available. Hysteresis in the relative permeability and capillary pressure relations arise because of the changes in intrapore fluid configuration (Aziz & Settari 1979; Lenhard *et al.* 1989a). As the change in fluid configuration cannot be described by the classical multiphase model field variables (saturations and fluid phase composition), additional empirical (and not self-consistently predicted) parameters are introduced to model the observed hysteresis (Parker & Lenhard 1987; Lenhard *et al.* 1989a). Progress in this area has been hampered by the absence of a complete set of variables to describe the pore-scale fluid configuration dynamics. Therefore, there is a need for a new multiphase flow formulation that is sufficiently comprehensive to self-consistently model the changing wetting and other pore scale fluid configurational variations (Ortoleva 1998; Tuncay & Ortoleva 2001).

Texture evolution models

Texture sits at the heart of many feedback processes and related coupling that underlie crustal system evolution. In this way, the dependence of many phenomenologic laws on rock texture couples all RTM processes. A complete model of crustal evolution must be based on a sufficiently complete set of textural variables and the equations yielding their dynamics. Including such laws in basin models allows the texture-dependent RTM process rate laws be continuously updated over the evolution period of interest.

We suggest that rigorous models of rock behavior should be of the Markov type – i.e. the rate of change of rock state should only depend on the instantaneous rock state and not on prior history. Stress and strain are related through rock rheology to rock texture Θ (grain size, shape, packing, mineralogy, and fracture length, aperture and orientation statistics). Pressure solution and grain breakage imply that the rate of change of Θ depends on stress, denoted σ. If Θ satisfies the differential equation $d\Theta/dt = G(\Theta, \sigma)$, then, in principle, $\Theta(t)$ is a functional of σ, i.e. depends on $\sigma(t')$ for all $t' < t$, $\Theta = \Theta[\sigma]$ As rheology depends on Θ, we see that $\Theta[\sigma]$ reflects the entire prior stress history and not just the instantaneous value of σ. However, this 'memory' in a theory wherein Θ is not coevolved with σ is an artifact of the incompleteness of the model. While there are many stress-strain histories that could lead to the instantaneous state of a rock, only the latter is key to predicting its failure and other behavior (Tuncay *et al.* 2000a; Tuncay & Ortoleva 2001).

Weyl (1959) proposed that a texture model was introduced based on a periodic array of truncated spheres. Dewers & Ortoleva (1990a,b,c, 1991a,b) showed how such a texture model could be used in an RTM model. They described the interplay of effect of diffusion and pressure solution to yield diagenetic bedding, stylolites, and related phenomena (see also Ortoleva 1994a,b, 1998 in the wider context of basin modeling). The limitation of this approach is that, with the exception of single grain plastic deformation (Dewers & Ortoleva 1991b), it cannot describe mechanical compaction through grain boundary slip or grain breakage. Furthermore, as it is limited to isogeometric deformation, it cannot account for nucleation, a range of particle sizes and the complex interplay between mechanical and pressure solution deformation in multimineralic systems. The incompleteness of existing texture models is a major drawback in quantitative basin modeling. Improved models would allow for the discrimination between rocks of similar grain size and porosity but of different origins (e.g. chemically precipitated versus mechanically deposited).

Faulting

The deformation of brittle rocks is a multiple time and length scale phenomenon. Rocks fail rapidly but heal slowly on geologic time scales (Logan & Teufel 1986; Fredrich & Evans 1992). Brittle rocks have two sources of memory. They store elastic energy, and, once failed, have broken grain–grain contacts and gouge that persist over long times. Viscous deformation or failure erase the former while chemical healing processes diminish or erase the latter. When sheared across a large-scale zone, rocks can fail within a meter-scale fault zone. Furthermore, the fault dynamic typically takes the form of a series of short time scale events with long inter-event healing periods to form the faulting cycle. The challenge is to develop a rheologic model of this deformation behavior that captures this multiple scale character autonomously – i.e. from an initially uniform, unfailed system to a faulted one, experiencing intermittent failure-healing cyclicity and complex spatial structure. Therefore, fault simulation must be carried out in three spatial dimensions via a model that incorporates a full suite of crustal RTM processes. A preliminary extension of a basin model to simulate faulting is presented by Ozkan *et al.* (1998) and Tuncay *et al.* (2001).

Organic geochemical kinetics

To attain predictability under a wide range of thermal histories and for kerogen of a variety of compositions, it is necessary to base a maturation model on the detailed chemical reaction network with associated laws guided by rules of organic chemistry. Most existing organic geochemical models are based on overall reactions, which do not capture the intermediate processes and are thereby difficult to calibrate in general (Tissot *et al.* 1987; Espitalie *et al.* 1988; Braun & Burnham 1990; Hunt *et al.* 1991; Pepper & Corvi 1995).

INFORMATION THEORY FORMULATION

A central challenge of basin modeling is to construct the present-day internal configuration and chronology of the subsurface from data of a range of types and quality, sparsely distributed across a study area. As the available data are typically indirect and fraught with uncertainty, an objective methodology is needed that yields the most probable chronology and present-day configuration as well as an estimate of the associated uncertainty. Further, there is often a great quantity of data that are too time consuming to be fully integrated by classical methods, and methods of analysis are often subject to individual bias. We now outline the MAI approach to the challenges of petroleum Exploration and Production (E&P) based on an information theory (probabilistic) integration of basin modeling and large databases.

Basin data must be integrated with modeling to compensate for the incompleteness of both. Furthermore, the integration must be automated, i.e. seismic, well-log, core and other data must, to the extent possible, be used as direct input to the model so as to reduce labor-intensive tasks and to eliminate bias in the interpretation of the geologic record. On the other hand, the automation should somehow integrate our geologic experience/expertise in a natural way so as to minimize the extent of the computations.

There are two main categories of factors that an automated procedure must determine to run a model. The first is the least well-known parameters in the phenomenologic expressions and, second, the scenario of factors influencing the basin at its boundaries (uplift/subsidence and compression/extension/wrenching; basement heat flux, climate, and sediment/erosion). The latter factors change across the basin's boundaries and over the history of the basin (see Fig. 3). Below we outline a new approach, presenting a derivation of an equation for the most probable history of the spatial distribution of the least well-constrained boundary factors. Having delineated these factors, one may use them with a basin model to estimate the time course of the internal state of a basin from the inception of a basin to the present. This approach has been demonstrated for an engineering problem (Tuncay & Ortoleva 2002).

Let B represent the time course of a set of influences acting on the basin boundaries (see Figs 2 and 3). Thus, B represents the histories of compression/extension and upheaval/subsidence or of other factors (basement heat and fluid flux, sea level, sediment input, erosion) acting at each point on the basin's top, side, and bottom. Let $\rho[B]$ be the probability of a given scenario B of these influences. For example, if B represents the basement heat flux at all points on the basin

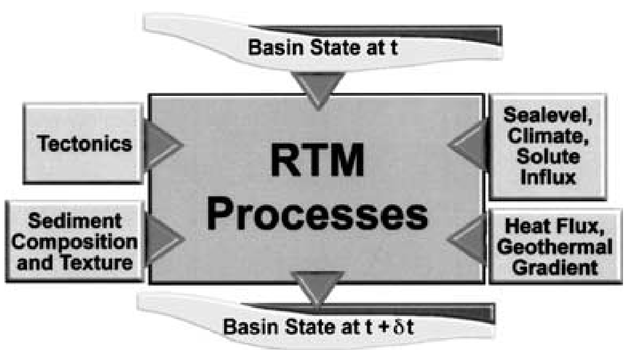

Fig. 3. Schematic flow chart showing how the interplay of geologic data and reaction-transport-mechanical process modules evolve the basin over each computational time interval δt.

bottom for all times of the basin's history (inception to present), then ρ depends on the infinity of these heat fluxes (all points on the bottom for all times). Let S indicate an integration of the infinity of such variables, i.e. a functional integral; then normalization of ρ implies

$$\underset{B}{S}\rho = 1. \tag{3}$$

Information theory (Jaynes 1957) in the present context is based on the entropy S defined via

$$S = -\underset{B}{S}\rho \ln \rho. \tag{4}$$

S is taken to be a measure of the uncertainty we have in the state of a system; thus as the number of possible states of the system increases so does the entropy. The probability ρ is determined to be that functional of B, which maximizes S subject to equation 3 and information we may have about the system (e.g. seismic, well-log, fluid pressure, core analysis, etc.).

Let $O^{(k)}$ be the kth set of the aforementioned data we have on the basin $k = 1, 2, \ldots, N_{\text{error}}$. Thus, $O^{(1)}$ could be a seismic survey on one area, $O^{(2)}$ a survey on another, $O^{(3)}$ is a suite of logs at various locations, etc. Similarly, let $\Omega^{(k)}$ be the synthetic seismic or other data as constructed using a basin simulator. With this, we construct the kth error $E^{(k)}$ defined such that

$$E^{(k)} = \sum_{j=1}^{N^{(k)}} (\Omega_j{}^{(k)}[B] - O_j{}^{(k)})^2 \tag{5}$$

As a basin simulation depends on B, then so does the synthetic data $\Omega^{(k)}$ constructed from it. In equation (5), $N^{(k)}$ is the number of data values of type k, $O_j{}^{(k)}$ is the jth value of type k ($j = 1, 2, \ldots, N^{(k)}$) and $\Omega^{(k)}$ is the synthetic value of $O_j{}^{(k)}$. With this, we impose the conditions

$$\underset{B}{S}\rho E^k = E^{(k)^*} \tag{6}$$

where $E^{(k)^*}$ is an estimated value of $E^{(k)}$ obtained from our general knowledge of the accuracy of the available data, numerical accuracy of the basin simulator, and the formulas used to construct $\Omega^{(k)}$ from it.

The spatial sparseness of the available data does not allow us to determine the spatial dependence of B on short length scales. Furthermore, practical basin simulation does not allow for very fine grid spacing. Thus, it is not feasible to seek a very fine spatial scale resolution of the B parameters. A similar consideration holds for the time dependence of the B parameters. To constrain the scale at which we wish to delineate the space–time variations in the state of the system, we impose the conditions

$$\underset{B}{S}\rho \int_0^{t_{\text{present}}} \mathrm{d}t \frac{1}{A} \int_{\text{boundary}} \mathrm{d}^2 r \frac{1}{2} |(\underline{\nabla} - \underline{n}(\underline{n} \cdot \underline{\nabla}))B_\alpha|^2 = \chi_\alpha \tag{7}$$

where t_{present} is the age of the basin ($t = 0$ being the time at basin inception), and $\underline{n}$ is a unit normal to the basin's boundary pointing outward; $\underline{n}$ and ∇ terms imply a tangential gradient. Similarly,

$$\underset{B}{S}\rho \int_0^{t_{\text{present}}} \mathrm{d}t \frac{1}{A} \int_{\text{boundary}} \mathrm{d}^2 r \frac{1}{2} \left(\frac{\partial B}{\partial t}\right)^2 = \theta_\alpha \tag{8}$$

In the above, B_α is the αth of the N_b boundary factors ($B = \{B_1, B_2, \ldots, B_{N_b}\}$) and χ_α and θ_α are estimates that constrain the spatial and time derivatives of B_α while A is the (time-dependent) surface area of the basin. The types of boundary factors we shall consider are $\alpha =$ basement heat flux, lateral boundary shape for compression/extension tectonics, shape of the bottom of the basin.

In the light of information theory (Jaynes 1957), we maximize S subject to the constraints (equations 3, 6–8) to obtain ρ, we find,

$$\begin{aligned} \ln \rho = -\ln Q &- \sum_{k=1}^{N_{\text{error}}} \beta_k E^{(k)} \\ &- \sum_{\alpha=1}^{N_b} \lambda_\alpha \int_0^{t_{\text{present}}} \mathrm{d}t \frac{1}{A} \int_{\text{boundary}} \mathrm{d}^2 r |(\underline{\nabla} - \underline{n}(\underline{n} \cdot \underline{\nabla}))B_\alpha|^2 \\ &- \sum_{\alpha=1}^{N_b} \omega_\alpha \int_0^{t_{\text{present}}} \mathrm{d}t \frac{1}{A} \int_{\text{boundary}} \mathrm{d}^2 r \left(\frac{\partial B_\alpha}{\partial t}\right)^2. \end{aligned} \tag{9}$$

This completes the formal construction of ρ (once the normalization constant Q is evaluated via equation (3) and the Lagrange multipliers (β-, λ-, ω-parameters) are fixed via equations (6–8).

The most probable space-time dependence of the B_α are determined to be those which maximize ρ. We find, upon setting the functional derivatives of equation (9) to zero,

$$\frac{\delta \ln \rho}{\delta B_\alpha} = 0 \; (\alpha = 1, 2, \cdots, N_b) \tag{10}$$

To find B, we shall solve this set of functional differential equations.

Our approach can be more explicitly illustrated for the most probable history of the basement heat flux. Let $B(x, y, t)$ be the vertical heat flux into the bottom of a basin at map view position (x, y) at time t. For the simple case of a single type of error E, we have

$$\beta \frac{\delta E}{\delta B(x, y, t)} - \frac{\chi}{A}\left[\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2}\right] - \frac{\theta}{A}\frac{\partial^2 B}{\partial t^2} = 0 \tag{11}$$

for area A of the basin bottom taken to be constant for simplicity of illustration here. This equation has the character of a space-time diffusional dynamic interacting with the nonlinear $\delta E/\delta B$ term that is a functional derivative of E with respect to $B(x, y, t)$. The $\delta E/\delta B$ term is constructed using a basin simulator.

In the approach presented above, two conditions (equations 7 and 8) are used to constrain the spatial and temporal resolution of the B parameters. The use of prior information to regularize the inverse problems is a common practice. This can be achieved through an additional error measure in the form of

$$E_\alpha{}^B = \sum_{j=1}^{M} (B_\alpha{}^j - B_\alpha{}^{jp})^2 \quad (12)$$

where M is the number of points used to discretize B, and $B_\alpha{}^{jp}$ is the prior information, which is usually taken as the initial guess. The use of prior information is convenient. However, it may also be misleading if it masks the observed data. An alternative approach to account for prior information is through the use of the minimum relative entropy principle (Kullback 1959; Kapur 1988; Woodbury & Ulrych 1996). The minimum relative entropy principle suggests that the probability ρ is constructed by the minimization of the functional H:

$$H = \underset{B}{S} \rho \ln \frac{\rho}{q} \quad (13)$$

with respect to ρ. In equation (13), q is the *a priori* probability distribution. The use of a quadratic error measure (such as equation 12) for the set of uncertain parameters corresponds to the assumption of a Gaussian distribution for the prior information. The minimum relative entropy principle allows one to tailor the *a priori* probability to the degree of uncertainty once has accumulated through the experience/expertise.

An approximation to ρ can be obtained by expanding equation (9) around the most probable B

$$\ln \rho \approx \ln \rho|_{\underline{B}^m} + \sum_{\alpha=1}^{N_b} \sum_{i=1}^{n} \frac{\partial \ln \rho}{\partial B_\alpha{}^i}\bigg|_{\underline{B}^m} \Delta B_\alpha{}^i + \sum_{\alpha=1}^{N_b} \sum_{i,j=1}^{n} \frac{1}{2} \frac{\partial \ln \rho}{\partial B_\alpha{}^i \partial B_\alpha{}^j}\bigg|_{\underline{B}^m} \Delta B_\alpha{}^i \Delta B_\alpha{}^j + \cdots \quad (14)$$

At the most probable scenario ($\underline{B}^m$) the second term vanishes. This approximate probability distribution accounts for all the available information, i.e. geologic data and associated error, *a priori* information, and regularization constraints for temporal and spatial distributions. The matrix of the quadratic term is constructed in the course of carrying out a large number of basin simulations to solve equation (10) numerically. Equation (14) is used to assess the uncertainty associated with the B parameters.

A flowchart for the information theory approach is shown in Fig. 4. Tuncay & Ortoleva (2002) presented preliminary results in the context of reservoir modeling using this approach.

CONCLUSIONS

The development of basin simulators has been influenced by several factors:

- availability of mathematical models to describe individual RTM processes;
- improvements in computer hardware;
- availability of efficient, stable and accurate numerical techniques; and
- interest and support by industry and government agencies.

While applied E&P teams have always been pressing for a basin simulator that can run on a PC in a short time, the reality is that accounting for the many RTM processes requires supercomputing power. While many research teams have attempted to develop simplified models, they have usually failed to communicate the likely pitfalls of an incomplete model. What needed are collaborative projects between industry, government, and academia that combine long-time scientific and financial commitments to make developments of comprehensive basin simulators feasible.

A serious limitation to the successful use of comprehensive basin simulators is the large amount of CPU time presently required for each simulation. This CPU time depends on the spatial dimensionality, spatial resolution, and the number of processes accounted for. The time/cost of the labor-intensive development of basin input data has also been a prohibiting factor in making comprehensive models effective, as has the difficulty in calibrating some of the phenomenologic parameters. Likely availability of faster CPUs and massive parallel architecture and algorithms as well as automated input data schemes based on information theory should accelerate these computations in the next 5 years.

Quantitative basin modeling provides several approaches to the goal of establishing steady and long-term petroleum through exploration and production technologies that utilize the computer-automated analysis of well-log, seismic, geochemical, and other data. Notable among the benefits of this MAI technology are the following:

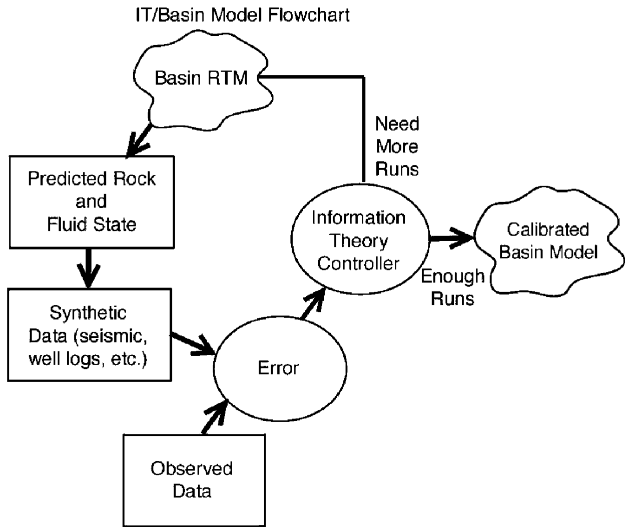

Fig. 4. This automated methodology is based on computational algorithm and I/O to yield the most probable state of the system given observed data and comprehensive physics and chemistry in the basin simulator.

- Improve the prediction of reservoir location and characteristics (fracture and matrix permeability, reserves in place, reservoir geometry, *in situ* stress, etc.) to lower the cost of exploration and production for deep reserves.
- Identify compartments and, thereby, locate by-passed resources.
- Make use of the billions of dollars of well-log, seismic, core, geochemical, and other basin data, which are presently under-used because of the cost of labor-intensive and often biased methods for interpretation.
- Use MAI-predicted reservoir characteristics to plan directions for horizontal wells and other factors to optimize field development and production.
- Achieve quantitative assessment of risk/uncertainty using an MAI approach.

At present, the total investment in basin modeling is a negligible percentage of even the most conservative estimates of the benefits that the comprehensive, MAI basin-modeling technology would yield. We conclude that more resources should be made available for the development of comprehensive basin simulators and MAI software in the near future so as to make the benefits of this technology available to the industry.

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