Sedimentary Basins as Thermochemical Reactors

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■ *The search for hydrocarbons has been one of the costliest enterprises of the 20th Century, yet there is still no surefire method for accurately predicting the specific location of oil and gas without drilling. This is because we still have a poor understanding of how, why and where oil and gas are trapped within a sedimentary basin. The Global Basins Research Network has constructed a "Data Cube" of a sub-basin in the Plio-Pleistocene Gulf Coast of the United States, containing internally consistent geophysical, geochemical and geological data relevant to fluid flow within a 60 km x 40 km x 10 km volume of Gulf Coast sediment. The Data Cube and a massively parallel, 3-D supercomputer model of the fluid flow history within the Data Cube will enable us to reconstruct the evolution of the whole volume as a* thermochemical reactor, *and thus to predict more accurately the final locations of its oil and gas.*

Great strides have been made in the past ten years in the understanding of the static processes of sedimentary basins in terms of the evolution of their stratigraphy, vertical tectonics and structure. However, sedimentary basins are beginning to be looked at as dynamic entities, as thermochemical reactors: complexly interrelated systems that are deformed and faulted by tectonic forces, modified by sedimentation and erosion, and dramatically influenced by fluid flow—which itself produces reactive chemical change. Indeed, it is the fluids flowing within basins that control the concentration and location of all our gas and oil deposits, as well as most minerals. But while we know a great deal about specific processes that contribute to and affect the production and migration of hydrocarbons, we don't yet have good models for describing and predicting the dynamic couplings between these major basin processes.

This is one problem that is too big for any one university or corporate group to solve (even by an oil industry lab), so Lamont-Doherty has joined a consortium of university and industry scientists from throughout the United States in setting up the Global Basins Research Network (GBRN), a remotely linked, interactive research organization.

The Gulf of Mexico

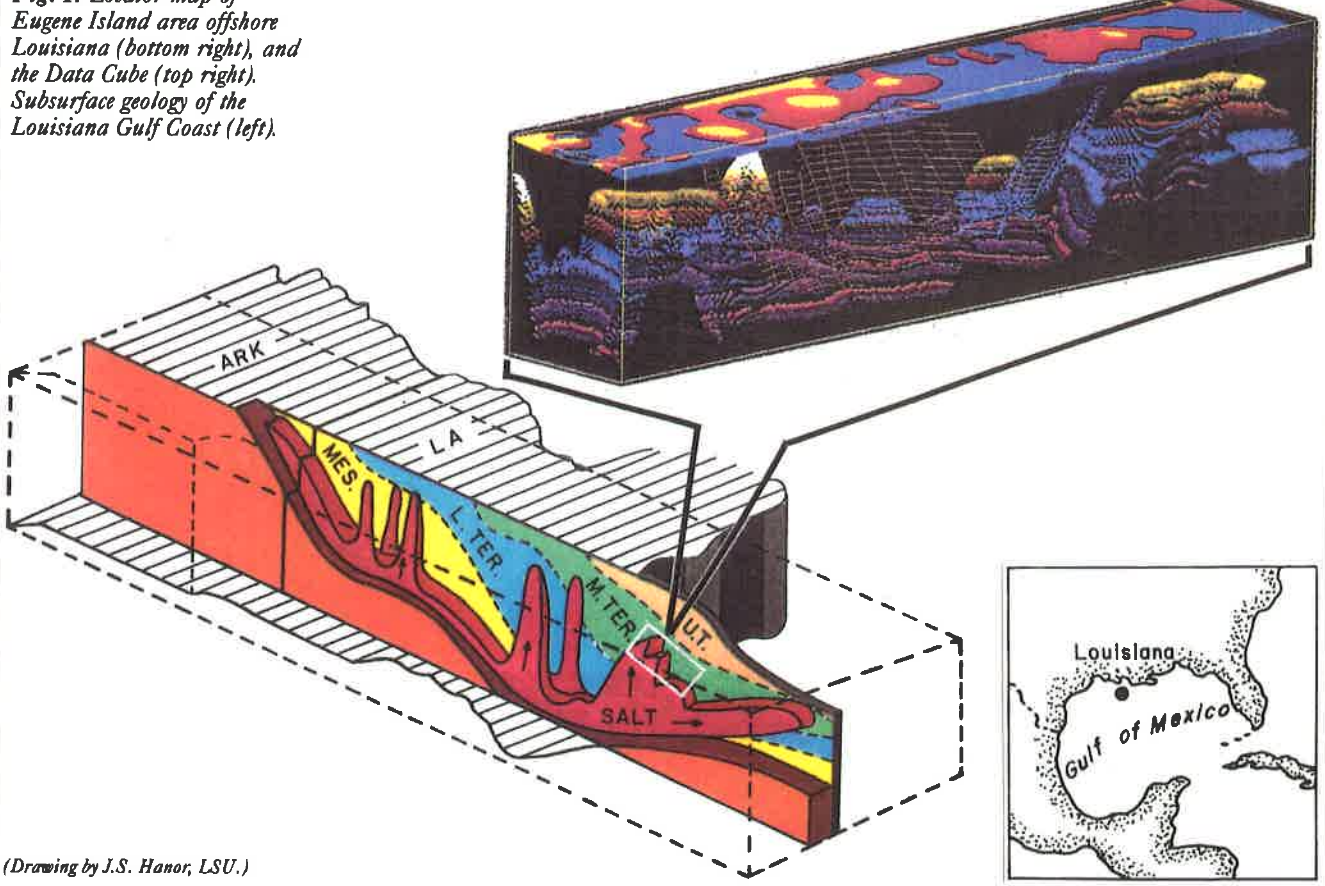
Our approach to investigating and modeling coupled basin processes as a single, unified system requires the development of new methods and techniques to identify and map the time-dependent dynamics of fluid movement. The ideal location for developing such technologies is a basin with presently active maturation and expulsion of hydrocarbons. So we chose the Plio-Pleistocene Gulf of Mexico as the initial focus of our research. The Gulf is the dominant hydrocarbon-producing province in the coterminous United States, and there is a wealth of geophysical and geochemical data from the basin. Over $100 billion has been spent in the exploration and production of oil and gas on this margin in the last twenty years alone. However, because of the recent movement of its phenomenal salt structures, the massive pile of sediments contributed by the Mississipi River in only the last few million years, and the relatively late maturation of its oil and gas, the Gulf basin is extraordinarily complex and extremely active.

We decided that before attempting to model the evolution and dynamics of the Gulf basin as a whole, we had first to establish a three-dimensional understanding of the physical and chemical parameters that control the dynamic processes of fluid flow in a smaller sector of the Gulf—the offshore Louisiana Gulf Coast, and particularly the South Eugene Island area. Containing the largest offshore oilfield in the United Sates, it is one of the best studied and most extensively sampled (but not yet synthesized) sub-basins in the Gulf—indeed, in the world.

The GBRN is now assembling seismic, surface heat flow, temperature, pressure, fluid compositions, cuttings and log information for this area. These data are being synthesized into a three-dimensional volumetric description of the subsurface, which we call a "Data Cube" **(Fig. 1)**. The Data Cube will enable us to describe and define the specific processes that are essential to constrain the coupled models that will determine how the sub-basin has evolved.

The geophysical evolution and structure of the Eugene Island area is quite well understood. Its sediment dynamics have not been affected greatly by recent basement tectonics. Significant sedimentation was delayed until well after the Jurassic rifting that opened the Gulf of Mexico. Abundant terrigenous sedimentation began only after the Laramide orogeny and the uplift of the Rocky Mountains. The delivery of the Laramide erosional products was further delayed by the lower Cretaceous barrier reef system that developed along the hinge zone of the Gulf. This reef prevented most erosional sediments from reaching the offshore basin, and as a result organic-rich, marine sediments were deposited without much dilution.

Fig. 1: Locator map of Eugene Island area offshore Louisiana (bottom right), and the Data Cube (top right). Subsurface geology of the Louisiana Gulf Coast (left).



(Drawing by J.S. Hanor, LSU.)

The Laramide sediments finally breached the reef in the Tertiary, and the ancestral Mississippi delta system dumped an enormous thickness of sediments into the Gulf Coast basin. The pre-Tertiary marine sediments were buried, loaded and heated with unusual rapidity. This rapid loading triggered the dramatic migration of the Jurassic Louann salt (which originated during dessication events associated with the initial rifting of Yucatan from Louisiana/Texas), and developed some of the most rugged topography on Earth. The Gulf Coast salt relief is the greatest on the planet, with the exception of cumulo-nimbus clouds and associated thunderheads. The massive dumping of all this sediment prevented normal dewatering and increased pore pressures within the deeper sediments to far greater-than-hydrostatic (geopressures), causing the maturation and migration of large volumes of hydrocarbons. All these changes continue to this day (see article by Karner *et al*, page 88).

Gulf Coast Hydrodynamics

We know from drilling data that large-scale hydrodynamic processes are coupled with the ongoing deposition of this massive sedimentary load. Convection is occurring in all three of the major hydrological regimes active in the Louisiana Gulf Coast. At shallow depths, meteoric flow, controlled by topography and directed toward the shelf, mixes with upward moving connate water and diagenetic fluids from deeper in the basin. At mid-depths, considerable dissolution of salt occurs, which produces an unstable layer of heavy, dense, and highly saline pore fluids. In the deepest portion of the basin, compaction and hydrocarbon maturation reactions release large volumes of high-temperature, geopressured, extremely buoyant fluids. Thermal build-up and restricted fluid flow are associated with the top of the geopressured zone, which dominates the deeper compactional system within the basin. Hydrothermal fluids expelled from the geopressured "chambers" are known to migrate both laterally and vertically for considerable distances in the Louisiana Gulf Coast region.

In addition to these subsidence- and chemically-driven hydrodynamic forces, the mountainous topography and movement of the hot salt itself results in tremendous thermal as well as hydraulic gradients over very short distances in the subsurface. The thermal conductivity of salt is five times that of sandstone, and ten times that of shale, so its location and movement will dominate the deep thermal structure of the basin. The high thermal conductivity of the salt relative to the surrounding sediments causes the refraction of tremendous quantities of heat away from the deep basin shales and toward the salt highs. Isotherms can even become subvertical near salt columns.

The form and magnitude of this hydrothermal and hydrodynamic fluid flow is controlled by both the buoyancy forces acting on the fluids (temperature, pressure, chemical gradients and fluid densities), and the permeability pathways available to the fluids. As in most geological situations, the predominant convecting fluid in the Gulf Coast is water — though oil, gas and saline brines are variously included.

The rate and duration of fluid movement in such a dynamic sedimentary basin is not slow and steady-state, but is transient and can be extremely rapid. Compaction and hydrocarbon generation create geopressures large enough to cause repeated hydraulic fracturing of the geopressured chambers. In turn this releases bursts of large volumes of water accompanied by oil and gas up the large growth faults and into overlying sediments. Similar transient releases of fluids from deep within geopressured chambers are thought to occur in many other hydrocarbon-producing basins elsewhere in the world.

The South Eugene Island Data Cube

From seismic reflection profiles, cutting analyses, and log data, we established salt topography and subsurface stratigraphic horizons, and these, together with the seafloor heat flow, were used to construct the Eugene Island Data Cube (**Fig. 2a**). The base is the top-of-salt surface, which was mapped from seismic profiles and verified by gravity observations. The complex red and blue grids are major normal growth fault systems; **b)** next above is a prominent sedimentary horizon above the salt, the Lenticulina (1) biostratigraphic surface (2.5 Ma), which is the base of the sand/shales sequence that is the primary hydrocarbon producer in this area; **c)** the top of this productive interval is the Angulogerina (B) biostratigraphic surface (1.5 Ma); and **d)** the upper boundary layer of the Data

Fig. 2

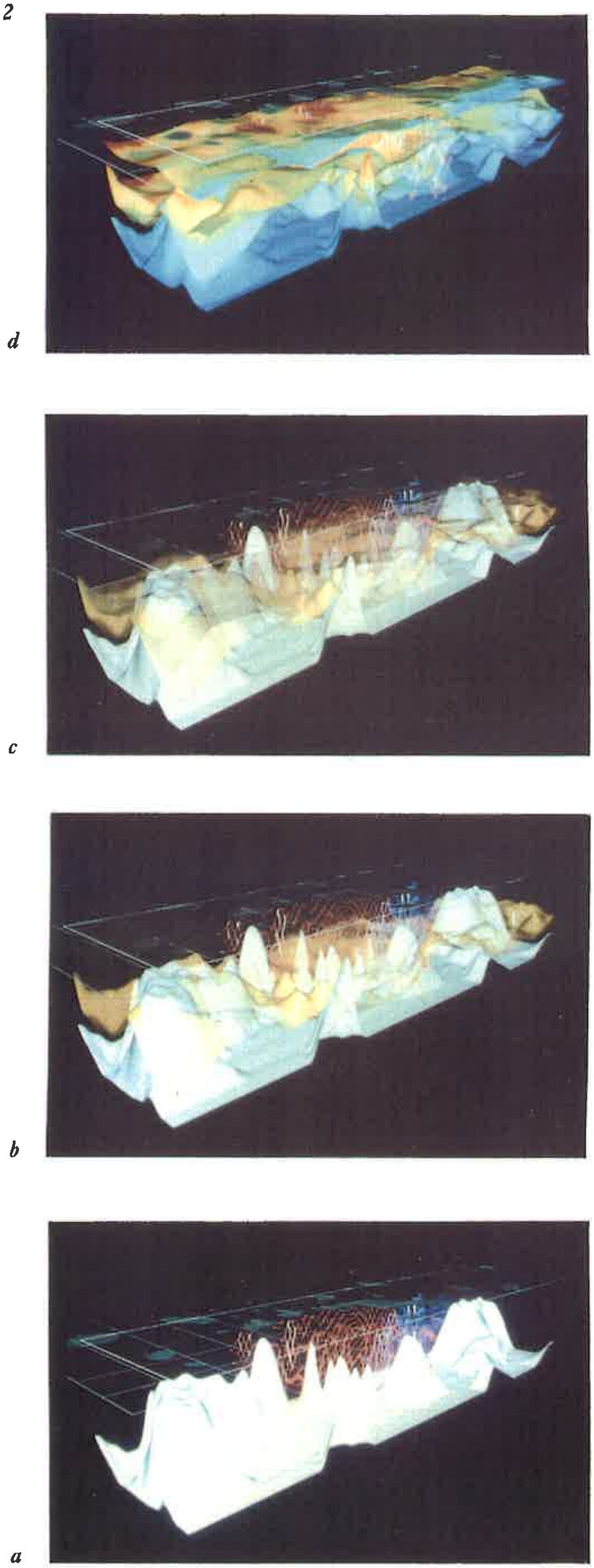


***Fig. 2:** The "Data Cube" is a three-dimensional synthesis of current geophysical exploration results and observations of the physical and chemical parameters that control the dynamic processes of fluid flow within a 60-km-long, 40-km-wide, 10-km-deep segment of the Eugene Island area of offshore Louisiana.*

*The Data Cube presently consists of structural and stratigraphic horizons defined from seismic profiles, surface heat flow, cuttings and log data: (from the bottom up) **(a)**: the extraordinarily rugged salt, with two growth faults (red and blue structures) that are clearly associated with oil and gas accumulation; **(b)**: the biostratigraphic Lenticula (1) (2.5 ma) horizon above the predominantly shale interval; **(c)**: the Angulogerina (B) biostratigraphic horizon (1.5 ma) at the top of the producing sand-shale sequence; and **(d)**: the distribution of heat flow at the seafloor surface.*

Cube is the distribution of surface heat flow.

Massive sands predominate from the seafloor to the Ang (B) surface, and geopressured shales are found predominantly from the base of the Lent (1) surface to the salt. Two of the many normal faults are shown by the Red and the Blue faults of **Fig. 2a.**

The plumbing system is complex: it distributes oil and gas rising from the geopressured shales into the more permeable sand intervals within the sand-shale sequence. Water accompanies the hydrocarbons upward, and moves into the even more permeable sands. The plumbing is actually upside-down, in that the most buoyant substances, the oil and gas, are trapped by the deepest water-permeable layers, whereas the water moves upward to flood the shallower sands.

This stripping of the hydrocarbons is somehow related to the major growth faults, since the oil and gas reservoirs are obviously related to them spatially. The faults are themselves quite complex. The blue one rides over the top of the salt ridge, and the red one bounds the oil and gas accumulations. But while the oil and gas are near the faults, they are offset from them. Production is in fact not along the faults, but among the deeper sand-shale horizons that abut the faults.

Heat Flow and Fluid Flow

The locations of oil and gas fields in the Eugene Island area are well known, but the controlling fluid flow forces that put them there are not well understood. The Data Cube horizons give us a static view of how the structure and stratigraphy might relate to fluid flow and to the movement of oil and gas, but we still need to define the physical and chemical dynamics involved. As a start, the GBRN has been mapping thermal and pressure surfaces, and analyzing their relationship to each other and to the stratigraphy.

Fig. 3

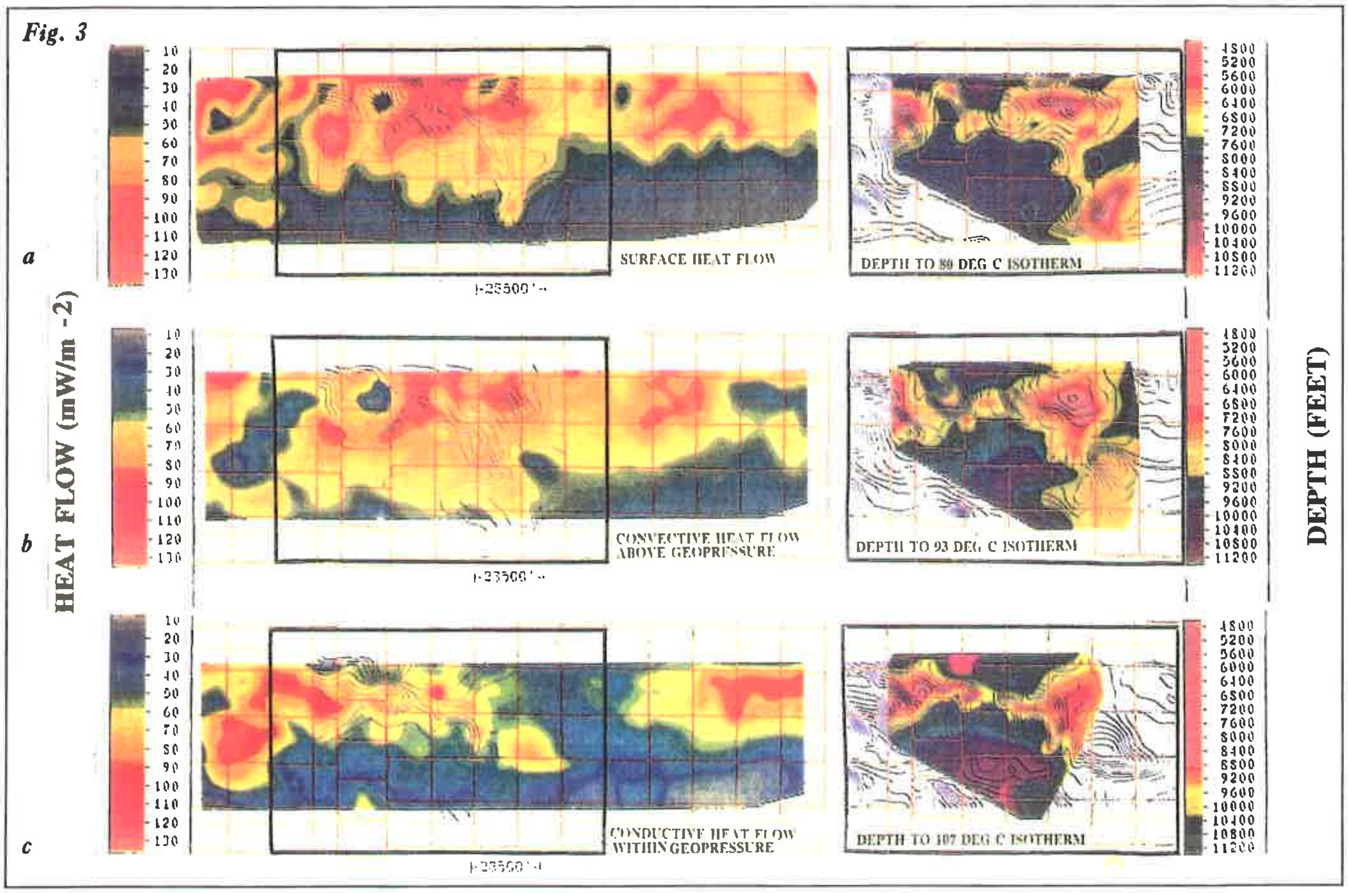


***Fig. 3a:** Surface heat flow (left) compared to the depth to the 80°C isotherm (right). Contours on each map are from the other. The 80°C isotherm is located above the top of geopressure surface, so movement of anomalies between this horizon and the surface must be due to convective heat flow, lateral thermal conductivity contrasts, and fault displacements within Pleistocene sands.*

(b): Convective heat flow calculated from the difference between the surface heat flow (top) and the heat flow conducted to the Lent (1) surface (bottom) compared to the 93°C isotherm. The 93°C isotherm is located within the transition from hydrostatic to geopressures, between the Ang (B) and the Lent (1) horizons.

(c): Heat flow conducted upward by the salt and geopressured shales to the Lent (1) horizon (left) compared to the 107°C isotherm, which is beneath the top-of-geopressure surface, and therefore should represent the thermal structure within the geopressured shales between the Lent (1) horizon and the top-of-salt.

Surface heat flow has proved to be an effective tool in scientific and geothermal exploration for interpreting subsurface fluid movements — but the technique has not been used at all in the oil industry. A high-density, surface heat flow survey was conducted over the Eugene Island Data Cube area by the Gulf Oil Company with the support of Lamont-Doherty Geological Observatory and this unique data set, since donated to Lamont by Chevron Corporation, provides a new and important dynamic observation for the investigation of the relationships among structure, tectonics, heat flow, and fluid flow in the Gulf Coast.

The heat flow surveying technique consists of lowering a vertical lance equipped with thermometers (thermistors) into the seafloor at periodic intervals. The thermistors measure the thermal gradient over the upper boundary layer of the basin (the upper few meters). After isolating the heat flux coming from within the basin from heat flow signals associated with oceanographic effects, we observed several high heat flow anomalies present across the upper boundary layer of the Data Cube. By combining the product of the measurements of the thermal conductivity of the surface sediments with thermal gradient, we were able to determine the heat flux from deeper in the basin **(Fig. 3)**. To prove the validity of the surface heat flow measurements, and to check for movement of heat in the subsurface, we checked the locations and magnitudes of the surface anomalies against a compilation of temperatures measured in 300 wells from a detailed study area within the Data Cube.

Conductive Heat Transfer

We set out to determine if the high heat flow anomalies we found at the upper boundary layer of the Data Cube were caused by upwelling within an active fluid flow system. More specifically, we wanted to determine the spatial relationship of these high surface heat flow anomalies to the salt topography (with its very high thermal conductivity), and whether the convective flow of hot fluids above the salt had displaced the thermal anomalies.

Conductive heat transfer theory predicts a strong spatial correlation between the tops of such massive salt bodies of extreme relief and high heat flow. (Within the Data Cube the salt topography has up to 20,000 feet of relief.)

We calculated the magnitude of the heat flow likely to be conducted through the top-of-salt and geopressured shales, and into the base of the sand-shale interval, the Lent (1) horizon (bottom surface, **Fig. 3c**). The difference between the surface heat flow (top surface, **Fig. 3a**) and the conductive heat flux likely to be exiting the geopressured Lent (1) layer was then calculated (center surface in **Fig. 3b**). This difference is assumed to be a *convective* heat flow surface just above the top-of-geopressure, and represents the heat transfer that cannot be explained by conduction.

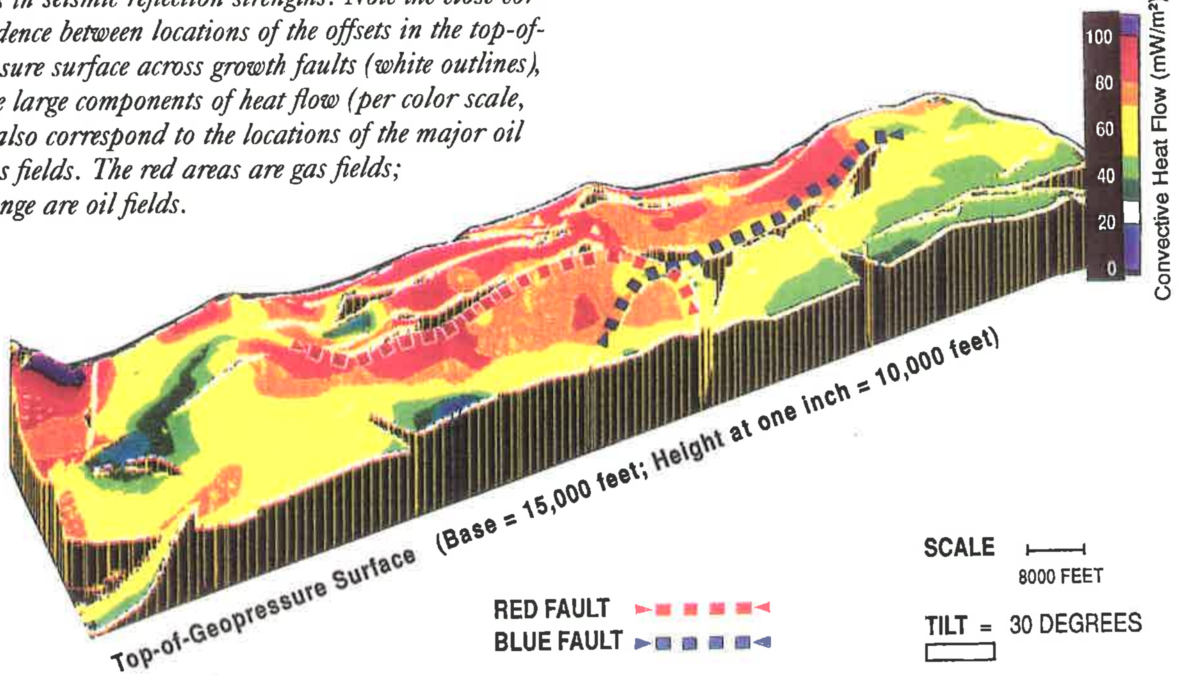
The convective heat flow surface quantifies the magnitudes and directions of fluid flow required to move the heat conducted from locations centered on the salt highs to the locations at the seafloor surface, where the high heat flow anomalies were measured. Thus the very displacement of the surface heat flow anomalies relative to the locations of the salt highs is a strong indicator that active fluid flow is presently occurring within the area of the Data Cube.

While a great deal of heat rises up the salt, the shales overlying the base of the salt have remarkably low heat flow (the purple area). In effect, the heat flow has bypassed those shales, leaving them colder than they should be at that depth. This has important implications for the timing of hydrocarbon maturation (see Karner *et al* article, page 88).

The Relation of Convective Heat Flow to the Top-of-Geopressure Surface

The most important dynamic boundary in the Gulf of Mexico is the top-of-geopressure surface. The transition zone from hydrostatic pressures above to those approaching lithostatic contains most of the hydrocarbon accumulations in the Gulf. This transition zone varies in thickness from a few hundred feet to several thousand feet, and is not a flat surface. In fact, it has been shown from well logs, mud weights and drill stem tests to have several thousand feet of relief in the data cube area. Using a novel seismic reflection strength mapping technique, the GBRN has shown the surface to be offset across the hydraulically important growth faults **(Fig. 4)**. More importantly, the convective heat flow anomalies from the completely independent geothermal data set correlate strongly with both the locations

Fig. 4: Convective heat flow (colors) projected onto top-of-geopressure surface (relief) derived from amplitude changes in seismic reflection strengths. Note the close correspondence between locations of the offsets in the top-of-geopressure surface across growth faults (white outlines), and the large components of heat flow (per color scale, which also correspond to the locations of the major oil and gas fields. The red areas are gas fields; the orange are oil fields.



of major offsets in the top-of-geopressure surface and the major locations of oil and gas accumulation in the Data Cube area. This suggests that the movement of hot fluids from the geopressure chambers upward along the faults is likely to be a signficant distributor of heat and hydrocarbons in the area.

Bursts Out of the Geopressured Shales

Fluid flow velocities of up to several meters per year, sustained only over a few thousand years, are required to account for the magnitudes of temperature anomalies observed in the Data Cube **(Fig. 5, Fig. 6)**. The intergranular permeability of sandstones in the Gulf Coast cannot support steady-state flow rates this high, and the volumes of fluid transport are also too great for steady state dewatering. Therefore the fluid flow must have occurred episodically, as "bursts" from the geopressured shales deep within the Data Cube area. That is, these very high fluid flow velocities can be maintained only with episodic opening of very high permeability pathways as a result of hydraulic fracturing. Preexisting growth faults can be hydraulically opened only when geopressures build to values that exceed the fracture reopening pressure in the Data Cube (the minimum compressive stress magnitude). Rapid bleeding-off of the geopressures quickly closes the faults again, but large volumes of hot fluid will have been released into the sand/shale sequence above **(Fig. 5)**.

As the water, oil and gas, accompanied by the heat, move upward, the oil and gas are stripped off into the first available space within the more normally pressured sands abutting the growth faults. The water keeps on moving upward, until it reaches aquifers in the sands. The heat continues to conduct and convect right up to the surface—where we can measure it.

The rapid thermal decay of transient heat flow events requires that the fluid bursts responsible for the high heat flow anomalies must have occurred within the last few thousand years in the Data Cube area of Eugene Island.

Three-D Finite Element Modelling

The Data Cube horizons give us an empirical, dynamic view of how the structure and stratigraphy relate to fluid flow and to the movement of oil and gas. The maps of thermal and pressure surfaces confirm their relationship to each other and to the stratigraphy. But we still have not precisely defined the physical and chemical equations involved, nor have we detailed how these coupled processes evolve. That is, we have not yet modelled the flow.

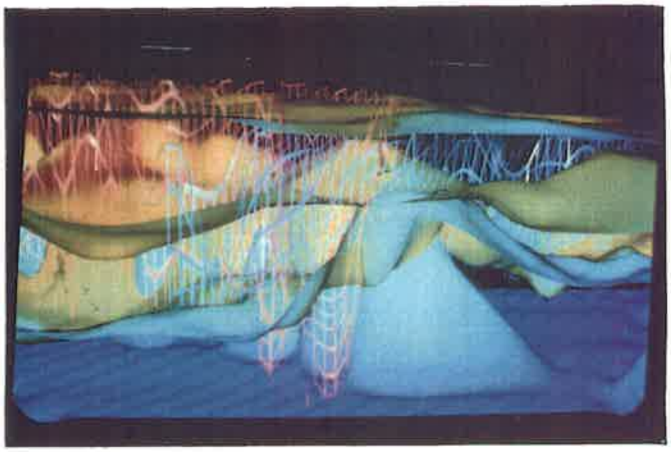
Basins begin to fill with fluid and sediment at rifting. With time, the coupled effects of sedimentation, compaction, heating, tectonism, and chemical alteration turn these water-filled sediments into rock, with the accompanying maturation and expulsion of oil and gas, as well as the displacement of much of the water. The permeability structure evolves with time, and is affected not only by changes in primary rock properties (porosity, mineralogy, lateral continuity of facies) but also by secondary changes such as diagenesis, faulting and secondary fracturing. Our successes in firmly connecting observed subsurface temperature flow to geopressures and episodic convection within the Data Cube make it clear that precise modelling of the flow of oil- and gas-saturated fluids is now possible.

The coupled equations describing fluid flow, temperature change, fault movement, chemical change, etc. have been cast in material coordinates and solved on the Cornell Theory Center supercomputer by a sophisticated commercial 3-D finite element code. The Computational Mechanics AKCESS.* code is unusual in that the differential equations that it solves are input as short (40- to 100-line-long) input files called templates. Component models (such as fluid flow or temperature) can be described by separate templates and solved simultaneously, with the terms that couple the equations calculated at each iteration or timestep.

Templates have currently been developed that describe and couple changes in 1) sea level, 2) sedipentation, 3) compaction, diapirism and faulting, 4) compactively-, convectively- and/or topographically-driven fluid flow, and 5) temperature. In the next year, salinity changes, inorganic chemical alteration, and organic maturation component models will be added.

These changes should enable the complete description of the processes occurring in the Eugene Island Data Cube. For example, the difficult numerical task of describing transient

Fig. 5a



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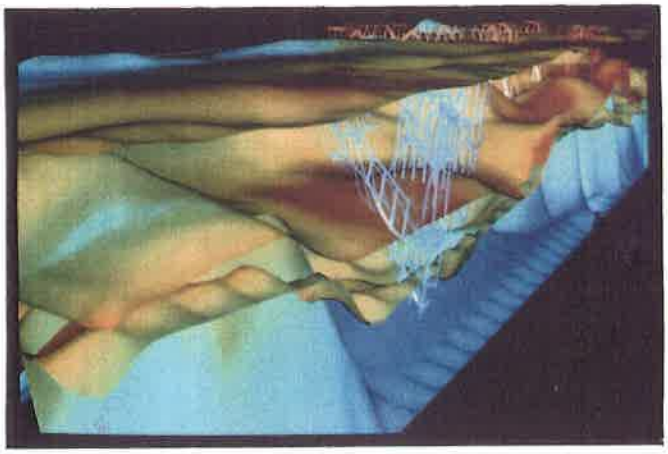

Fig. 5a: *Rotated and close-up of Data Cube, to south view along Red/Blue faults intersection. Note heat (red) corresponds to red Fault intersection with the top-of-geopressure surface (second down from top). The stripping of the hydrocarbons is directly related to the faults. But while the oil and gas are near the faults, they are offset from them. Production is in fact not along the faults, but among the deeper sand-shale horizons that abut the faults.*

Fig. 5b: *Rotation of Data Cube and close-up view from NW down the Blue fault. Note red heat along the Blue fault's intersection with the geopressure surface (second surface down).*

bursts of fluid has already been modelled in 2-D (**Fig.6**).

Summary

The goal of the GBRN is to compile comprehensive data on a representative portion of the Gulf of Mexico basin, and to make this data available on line to all the GBRN research institutions on modern workstations. The workstations are the tools that allow construction, visualization, and interpretation of the Data Cube, and they allow the interaction of model results and observations in the complex, multidisciplinary combinations that represent geologic reality in actual basins.

Over the next year or so the GBRN will work toward simulating the recent evolution of the South Eugene Island area described with increasing richness by the Data Cube. When the model is ready, results will be transmitted in real time to all the collaborating institutions and displayed on their workstations, using X-windows. In this way the model runs will be closely monitored. If parts go astray, the run can be aborted or corrected in mid-course.

In the largest sense the GBRN is pioneering the use of a network organization for carrying out scientific research. If the GBRN can make a significant contribution to basin modelling, the efficacy of a network research organization will be clearly demonstrated. Our narrower scientific aim is to deliver a "proof of concept" demonstration that specific sub-basins can be modelled in sufficient detail to predict the history of fluid movements and the locations of mineral and hydrocarbon resources in a way that is of practical use in exploration and production. Fluid flow modelling promises to be the best means of predicting the locations of oil and gas before wells are drilled. This approach perhaps portends the discovery of an entirely new generation of oil and gas in the thermochemical reactors we call sedimentary basins.

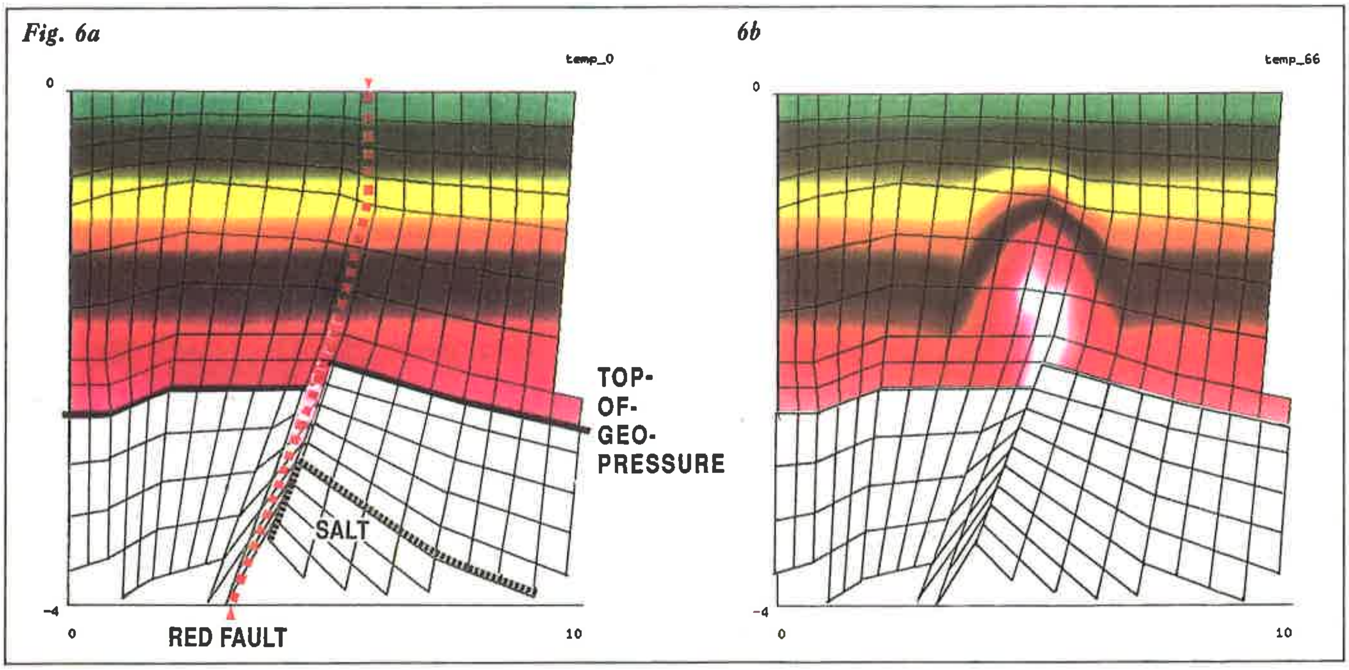

Fig. 6: *Fluid flow modelling within the structural, stratigraphic and dynamic constraints of the Data Cube requires parallel processing of a Finite Element code at the Cornell National Supercomputer Facility.*

(a): *Temperature at equilibrium at the beginning of the model run: time 0. A node at the intersection of top-of-geopressure surface and a growth fault is "opened" by instantaneously increasing permeability from 10^{-7} to 10^{-2} darcies.*

(b): *The fluid pulse is released upward along the fault (at 1 m/yr darcian velocity) where the most buoyant fluids (oil and gas) fill the first lower-pressure sands encountered. Note the leftward kick in the thermal plume caused by horizontal fluid injection. (This then becomes a major future oil reservoir.) Temperatures shown are at the 66th iteration (about 2000 years after the pulse is released).*