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**Submitted By
Timothy A. Cross,
Conference Convenor**

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22

REPORT OF WORKING GROUP 1 (2/18/88)
Philosophies guiding QDS model development: variables, scales and scope

Group Members: Mark Baker, Eric Barron, John Harbaugh, Bill Hay, Terry Jordan, Dave Lawrence, Margaret Lessenger, Ian Lerche, Katie Joe McDonough, Mark Sonnenfeld, Doug Waples

Philosophy

*We dreamed of a world systematic,
Finding patterns would make us ecstatic.
We quantified systems,
And shared algorithms,
While searching for models stochastic.*

*In the boondocks Tim made us convene,
Flaunting models for all to be seen.
But the lack of consensus,
Just served to incense us,
Teeth-gnashing and venting our spleen.*

*We waxed philosophic on sandstones
Over Baronet's protests and moans.
Jargoning for position,
(An old geo-tradition),
The clastickers sat chewing their bones.*

*We brought to Lost Valley our queries
Of Ian's equations and theories.
Somewhere on the road,
Zeitlin wrote the code,
While kissed by the muse of draft beeries.*

*And finally a model empirical
Which made all the world seem heuristical,
"It's chaotic!" was shouted,
(But still it was touted.)
That it functioned at all is a miracle!*

*And now my quantitative friends,
We've come to our dynamic end.
Our first QDS,
A raging success,
Go home and continue the trend!*

-- Katie Joe McDonough and Doug Waples

I. Fundamental and Empirical Laws

Categorization of laws either as "fundamental" or "empirical" does not appear to be a useful classification for quantitative simulation models. Fundamental and empirical laws are not antithetical, as most "fundamental" laws are firmly based on empirical validation. In deference to common usage, though, we allow that laws defined through empiricism need not be called empirical laws.

To clarify our terminology, we have defined four categories of relationships used in simulation modeling. These relationships are termed (1) fundamental laws, (2) first-order approximations, (3) empirical laws, and (4) gross empirical relationships. These four categories constitute parts of a continuum that ranges from fundamental to empirical.

Fundamental laws are those relationships that only scientists with divine pretensions would dare deny. These include, for example, the conservation laws and the laws of thermodynamics. It would be highly undesirable to permit a model's states to violate these laws by more than the levels of uncertainty in the measurable processes.

First-order approximations are those relationships of general applicability, directly related to model processes. These relations only approximate the complexity of physical systems, yet are often the most coherent, comprehensive, and internally consistent laws available. Examples include the diffusion equation, Darcy's law, and equations of chemical equilibrium and kinetics.

Empirical laws, also termed scientific generalizations, are those relationships of limited applicability based either on observed patterns or on imperfect understanding. Examples include compaction rates, and carbonate productivity rates as a function of environmental parameters.

Grossly empirical relationships are numerous and diverse. One form consists of linear approximations to relationships that are known to be nonlinear, such as the relationship between neutron log porosity and true porosity. Another such form consists of noncausal relationships such as a correlation between sunspot cycles and mosquito fertility as a factor in the demise of the dinosaurs. An example of still another form involves use of geometric relations as the basis for stratigraphic models, instead of more general first-order approximations.

There is a wide variety of scales and complexity of quantitative models, perhaps each using a different mixture of the various categories of laws. Generally any increase in scale, space, time, or number of state variables, is a product of increased complexity and requires a greater use of scientific generalizations and empirical relations. However, a major advantage of quantitative simulation models is that the fundamental conservation laws are still enforceable regardless of scale or complexity.

As a policy, models should incorporate relationships that are as fundamental as feasible. Initial stages of model development may require empirical relationships, but ideally a model's evolution should move toward use of progressively more fundamental relationships.

II. Role of Simulation in Developing Hypotheses

The primary task in developing simulation models is to simplify the complex natural system being represented, while still incorporating all important processes and feedback mechanisms necessary to the system representation. The objective is to develop quantitative tools that provide insight and which guide the course of scientific inquiry. Model simulations should be viewed as a form of scientific experimentation, that helps to test ideas and to develop and to better formulate hypotheses.

First, the development of models requires that concepts be expressed as equations, logic operations, and sequences of instructions. This task alone may provide added insight by focusing our attention on the components of the natural system, including those that can be stated readily, as well as on those components that are insufficiently known and require improved definition.

Second, it is likely that a set of equations developed to represent some complex natural system may be non-linear. Consequently, the behavior of the model of this system is unlikely to be appropriately represented by "summing" its components, nor is it likely to be deduced from purely conceptual descriptions of cause and effect relationships. Quantitative models are likely to illustrate interdependencies that might otherwise be obscure, their use may also lead to results that are not intuitive.

These two important aspects of simulation models and model development illustrate the integral role of quantitative approaches in testing ideas and in developing hypotheses. These benefits can be realized relatively early, and can provide heightened insight at all stages of hypothesis development. Models and model development are natural elements of the scientific method. The very complexity of natural systems suggest that models will always be interim in form, as any specific model is unlikely to represent a complete understanding of a natural system. Thus, the objective of employing simulation models is achieved if they serve as tools to formulate our ideas and sharpen our thinking. This objective requires a continual search for improvement, and involves devising and testing of algorithms, comparing results with observations, and formulating, revising and discarding models, or components of models in an effort to develop mature hypotheses that may guide further investigation.

III. Simulation and Education

Modeling should be incorporated routinely in academic courses at beginning undergraduate, advanced undergraduate, and graduate levels. They provide major advantages in demonstrating geologic processes in action, and in illustrating cause and effect relationships. Through simulation, students can be thrust into the role of working scientists as they develop, test, and modify hypotheses.

The effect of such exposure at the beginning undergraduate level should be to stimulate critical thinking, to develop problem-solving abilities, and to excite students about geology by showing its dependence on dynamic processes. Even students who do not become geologists will acquire skills that can be applied in other disciplines.

Upper-level undergraduates and graduate students could develop an enhanced appreciation of the sensitivity of geologic processes to changes in physical, chemical, or environmental parameters. This

appreciation should in turn enable them to understand natural variation in geologic environments in the modern world, and emphasize the limitations in interpreting the geologic past. Further more, the relationships between processes and components, and the importance of feedback mechanisms would be emphasized. Modeling will also aid in combining concepts derived from different courses, such as structural geology, sedimentology, and paleontology. Graduate students then would be prepared to use modeling procedures where appropriate in their thesis research.

Computers for such instructional use must be interactive and provide graphic displays for results of the simulations. Appropriate computer systems and information links already exist in many geoscience departments.

Many suitable software programs are also already available, although some modification may be necessary for didactic purposes. New programs are continually being developed and released to the public. The Journal of Geological Education is a source of such programs, and other clearing houses have been established.

IV. Scales and Boundaries

The temporal or spatial scale employed within quantitative stratigraphic models may vary by as much as 15 orders of magnitude. For models encompassing the stratigraphic response to long term climatic changes, the spatial upper limit may be the entire earth/solar system. Conversely, the reservoir engineer may be interested in simulating the permeability distribution and pore-throat geometry within a single bed of limited lateral extent and thickness near a development well. The scale chosen for simulation modeling should be application-driven. In terms of the petroleum industry, we may expect reservoir, prospect, play, basin, regional, and global-scale models. The temporal scale may vary from simulating flow events of a few seconds duration, to simulating the paleogeographic evolution of the entire Earth for the entire Phanerozoic.

In general, the scale and expanse chosen for simulation needs to be greater than the dimensions in time and space of the feature of interest. This provision minimizes problems with boundary conditions such that the model's performance is stable throughout the region of interest. As a corollary, grid and node spacing within the model must be less than the dimensions of the feature of interest, so as to avoid problems with aliasing. For example if sand distribution is to be modeled as a function of 100,000-year variations in sea level within a basin of complex bathymetry, the time interval chosen must be small enough to encompass variation within the 100,000 year cycle, and the spatial grid must be smaller than the size of the smallest bathymetric feature of interest.

In many applications, a hierarchy of scales will need to be established. For example, a geologist modeling gross shoreline trends on a play scale, may need to incorporate a subsidence component that is consistent with a basin-scale thermo-mechanical model. Forward models whose goals are stratigraphic simulation may be represented by a nest of spatial scales, each scale appropriate to one or more independent forcing functions. Examples of certain phenomena and the scales appropriate to them are given below, forming a nested sequence ranging from large to small:

<u>phenomenon</u>	<u>space</u>
climate	global or ocean basin
ocean currents	global or ocean basin
eustasy	global or ocean basin
subsidence history	tectonic province or lithospheric plate
sediment source history	drainage basin
sediment texture	river channel, submarine bar, etc
reservoir fluid flow	bed continuity & thickness.

At the boundary between lesser and larger scales, the larger scale dictates the boundary conditions for the smaller scale. Although the model may be operated on one of the smaller levels in the nest, any dynamic components of the model should be initiated in a manner that is consistent with the enclosing levels of the nest. Equations, algorithms, and parameters should be consistent at all scales within the model.

Finally, in many applications, the scale of the model will be dictated by data availability. Whenever possible, however, the model boundaries should be defined so as to coincide generally with natural boundaries.

V. General Requirements of Quantitative Models

- A. A crisp statement of the problem being addressed must be provided as a guide in constructing a model.
- B. All extrinsic and intrinsic assumptions, approximations, and limitations must be stated clearly before constructing or operating a model.
- C. Checks should be undertaken to ensure that the assumptions, axioms, approximations, and equations incorporated in the model are self-consistent.
- D. Initial values and global boundary conditions must be provided and checked for consistency with point 3.
- E. At the algorithmic stage, the local time-step conditions and the internal boundary conditions at spatial grid locations, as well as time steps and grid spacing, must be chosen for numerical stability, accuracy, and precision in a manner consistent with requirements of the basic statement of the problem as represented in points 2, 3, and 4.

VI. General Rules for Development and Operation of Quantitative Simulation Models

The use of models to investigate geologic systems is governed by three limitations. First, a model is a simplified representation of a complex system. Consequently, some uncertainty will exist as to whether all important processes and feedback relationships have been correctly incorporated. Second, the nature of geologic boundary conditions, and the external factors that influence geologic systems, may be uncertain. Third, the observations that characterize components of the geologic system are unlikely to be comprehensive, nor are they subject to unique interpretation. These limitations, and the philosophy of utilizing models as quantitative tools for insight, define rules and the guiding principles in the use of models.

First, the use of a hierarchy of models, from simple to complex, often maximizes insights into complex systems and focuses attention on the needs for future investigation.

Second, sensitivity analysis or experiments help define a model's interactions and interdependencies, and provide a clearer understanding of the model's response. In performing sensitivity experiments, it is essential to change only one variable at a time. In any complex interacting system, a change of more than one variable at a time may yield results for which the influence of the variables cannot be determined.

Third, if the model is extended, sensitivity tests with the extension's influence set to zero should be constructed to ensure that incorporation of the extension has not altered the model's performance with regard to its previous performance.

REPORT OF WORKING GROUP 2 (2/18/88)

Selection of variables for models of varying scales, scope and purposes

Group Members: Bob Goldhammer (Moderator), Andy Anderson, Bob Anderson, Scott Bowman, Walt Dean, Felix Gradstein, George Klein, Dave Swetland, Julian Thorne, Doug Williams, Dave Witter

Goal of QDS models for the next five years:

A goal of basin models for the next five years would be to generate reasonable forward models that can reproduce lithologic data interpreted from well logs. Ideally, we would like to have a model which will correlate and interpret seismic, well log, paleontological, geothermal, and geochemical data in its results.

Sedimentary and geomorphological processes are not tied well to dynamically defined processes. We are not able to address stratigraphers' needs at proper spatial/temporal relationships. The present geomorphologic models are advanced enough to get us into trouble. They may provide us with relationships which may appear convincing yet not represent reality. Most contemporary models have not incorporated some of the most basic empirical equations available.

I. Processes

The results of contemporary QDS models indicate that they can be successful at representing geologic processes on a large scale. However, no models represent actual physical, chemical processes which accurately portray sedimentary processes. Models are highly empirical; geometric, accommodation-space models; they crudely lump actual processes into gross results. Models are scale-dependent both temporally and spatially. Sedimentologists and geomorphologists need to know the temporal and spatial steps required by the limits of modern stratigraphic models. They are encouraged to stretch their process

models toward these larger scales. Their end product should be made as usable as possible to the stratigraphic modeler. A mathematical distillation of the amalgamated result of these longer process-geomorphological runs should be made, and contain input parameters which are related directly to the intrinsic, fundamental forcing variables.

Are we doing better with physical and chemical processes? This depends on who you talk to.

II. Variables - Our shopping list for sedimentary models

- A. Weathering rates -- a function of lithology, vegetation, and climate (gas, fluid, solid, and temperature). Status: Poor
- B. Erosion Rates -- a function of fluid flux, gravitational potential (slope, relief, etc.): channel and hill slope processes as a function of climate. Status: Fair
- C. Sedimentation -- Transportation and storage of various grain sizes as a function of local subsidence rates, fluid flow, climate, mineralogy and provenance. Distribution and velocity of fluid circulation as a function of basin configuration, tidal currents, and wave generation potential. Distribution of chemical elements within the basin. Chemical controls on sedimentation. Biogenic controls on production rate. Grain size variance as a function of depositional environment. We need to understand the relationship of sedimentation scale processes with an improved understanding of stratigraphically defined packages. Status: Fair to Poor
- D. Tectonic controls -- tectonic setting (passive margin, foreland basin, etc.) distribution, rate, and distribution of basement movement. Thermal and mechanical state of the basin. Status: Fair to Good - setting dependent
- E. Relative sea-level changes -- rate, magnitude, periodicity, and controls on changes in sea level. Need further research is needed on the apparent connection between genesis and temporal duration
 - i) Glacial eustasy -- Milankovitch cycles. Status: Good - Fair (some time periods need more definition)
 - ii) Evaporite driven eustasy. Status: Good
 - iii) Stress induced sea-level changes. Status: Good
 - iv) Major plate breakups and rearrangement, associated stress field changes. Need to stress genesis between lithospheric and external control. Status: Poor
 - v) Changes in rates of MOR spreading. Status: Good
 - vi) Increase in flexural rigidity through time within passive margins. Status: Poor
 - vii) Changes in age structure of the oceans. Status: Poor
- F. Diagenesis -- thermodynamic, kinetic controls on water rock interaction. What are the diagenetic controls on porosity and permeability. Need to effectively integrate diagenetic factors into QDS models. Need to differentiate between early and late diagenesis. Status: Poor
- G. Fluid flow -- rates of flow throughout the basin. Stability of flow. Interaction with thermal structure of the lithosphere. Pathways of flow as a function of porosity and permeability. Status: Good

III. Verification

- A. Framework -- A fine scale time-stratigraphic framework must be established. Once this is established, we can use this framework to compare with model results and constraints, and fine-tuned model variables.
- B. Facies models -- Facies Models must incorporate physical variables which control their formation. These physical parameters can then be used within QDS models.
- C. Paleo water depth -- The least explored variable in basin models is paleo water depth (PWD). Photic zone PWD can easily be assessed back through time with sufficient confidence. Unfortunately the same is not true for PWD in excess of 200-500 m, which is increasingly difficult to estimate with distance back in time, starting from the recent we recommend that paleontologists that generate age of PWD data in boreholes, combine this data in simple burial plots (age/depth) to see if their interpretations are geologically reasonable.
- D. New biostratigraphic techniques -- Conventional biostratigraphy in cored borehole or outcrop sections can generally resolve 1-2 Ma intervals, in exploration boreholes this resolution is 2-5 Ma or less. Probabilistic sequencing techniques (like RASC) increase resolution for detailed local correlation and calculate error bars on isochron. Conventional zonation/correlation should include judgement factors to be bundled for error bar analysis. Isotope geochemistry in selected basin with a well preserved carbonate record may resolve 20 ka time slices for the last 5 Ma or more. In high energy shallow marine environments, temporal resolution is less than in deep marine (slope) environments. It is the former that are most frequently modeled.

We recommend that stratigraphic test holes publicly available are executed in many basins in different tectonic settings in which modeling will play a role to understand geological history. It is critical that test holes access active margins and different coastal shelf systems tracts. These test areas model all different coastal shelf regimes (where we lack system tract data) and tectonic settings. These test holes should systematically sample and model the variability of both tectonic margins and styles, as well as systems tracts in different physical oceanographic regimes (such as macro tidal and tide-dominated areas and slopes).

IV. Communication

We need a 2-way transferal of knowledge and data from modelers to stratigraphers for the purpose of data collecting (i. e. isotope geochemical and biostratigraphic data). The communication will only be successful if there is a symbiotic relationship between modelers and data producers.

V. QDS Data Clearinghouse -

We recommend that a stratigraphic data clearly house (SDC) be established with the following goals: Access to global stratigraphic data in digitized format in accordance with the long-lasting example of the successful international seismological center.

REPORT OF WORKING GROUP 3 (2/17/88)

State-of-the-art in evaluating QDS models with stratigraphic information

Group Members: Peter Goodwin (Moderator), Frits Agterberg, Sam Butcher, Marc D'Iorio, Bill Galloway, Mark Hanson, Robert Laudati, Naka Nakayama, Chris Paola, Randell Stephenson, Lynn Watney

- I. The Process of Verification
 - A. Basic to the verification process is an understanding of the purposes of modeling. Purposes include:
 1. To test and quantify a concept or qualitative model
 2. To conduct sensitivity studies (experiments)
 3. To provide insight for further study and direct new and different observations
 4. To make predictions
 - B. Each quantitative model to be verified is a unique effort to explain quantitatively a particular geologic situation or set of observations behind which is a qualitative stratigraphic model. Therefore the first step in "verification" is to develop a thorough understanding of the quantitative model itself including its purpose, origin, structure and assumptions. The process of verification (validation, revision, falsification) is only as good as the geologic thinking behind the model itself.
 1. The more specific the geologic situation to be modeled and the more precise the process connection between the model and the situation, the greater is the potential for meaningful verification.
 2. Discrimination in scale between sedimentologic processes (e.g. transport, depositional and early diagenetic) and stratigraphic processes and input parameters (boundary conditions) is essential.
 - C. Tests of verification must be designed to gather data in forms specifically related to the model itself. Data currently in the literature are inadequate for testing new models. Because models dictate observations, the current literature contains data gathered under and in support of old models. New models require new data and new formats for expressing data.
 - D. Tests designed to falsify models need to be run. Scientific hypotheses are not verifiable; rather, hypotheses are considered scientific if they are capable of being falsified. Verification or falsification may be evaluated by:
 1. Internal consistency
 2. Basic compatibility between predictions of the model and observations of the stratigraphic record
 3. Condition of sufficiency
 4. Condition of necessity
 5. Increased confidence of model predictions through blind testing
 - E. Basic compatibility between predictions of the model and observations of the stratigraphic record constitutes a first approximation of verification. However, anomalous data and apparently

stochastic patterns not in direct conflict with the model should be the springboard for model refinement.

- F. The refined model should then be applied anew to the stratigraphic record as a more detailed test.
- G. Thus "verified" models have both a predictive role and a directive role providing us with insight for further study.

II. Stratigraphic Data Needs

- A. A fine-scale time-stratigraphic framework is essential to verification of all QDS models. We need to develop first on a regional basis and then globally, a framework for correlations and sea-level curves at Milankovitch scales (equivalent to 4th- and 5th-order cycles).
- B. Issues for immediate interdisciplinary attention
 - 1. Testing the Exxon sea-level curves and applying them to outcrop studies.
 - 2. The relationship between seismic sequences and small-scale cycles defined largely from outcrop studies
 - 3. Discriminating the specific contributions of tectonism and eustasy to the stratigraphic record
 - 4. Analysis of unconformities and condensed sections
 - 5. Relationship of traditional correlation techniques (e.g., bentonites and "key" or "marker" beds) to a cycle or sequence stratigraphic framework
 - 6. Relationship of biostratigraphic zonations to cycles and their bounding surfaces
 - 7. Allogenic versus autogenic cycles and surfaces
- C. The common thread of most of these issues is the discontinuous nature of the stratigraphic record at many scales. Given this structure to the record, we see the need to focus future stratigraphic studies on surfaces of discontinuity (e.g., cycle or genetic sequence boundaries and unconformities). The origin of these surfaces, their extent and particularly their significance as the physical framework for facies analysis are essential to verification studies. Stratigraphy of the past has been involved mostly with rock bodies; we see the immediate future of stratigraphy as being linked to the analysis of time-stratigraphic surfaces which constitute the temporal and spatial fabric of the stratigraphic record.

III. Data requirements for testing and refining sedimentologic data.

All of us agree that the advent of quantitative stratigraphic models could bring with it a *renaissance* of studies of recent sedimentation, with a new emphasis on quantitative studies of both processes and preserved sediments. We note that integrated quantitative studies of this type are not yet available in the literature although the recent CODE study of shelf transport comes close to what we have in mind.

- A. Basic Idea What we need are studies of sedimentary processes at time and space scales an order of magnitude larger than those attempted so far (e.g. studies of flow and sediment transport for a few days around a single channel bar). Such studies need to be done in areas of active rapid sedimentation, and they need to be coupled with ultra-high resolution stratigraphic and sedimentologic studies of associated recent sediments. The stratigraphy should be based on cores spaced closely enough to resolve all major facies types, dated with C¹⁴ and chemical means, and on high-frequency seismic. It is absolutely crucial that the process data be obtained during "record-forming" events (floods, storms, etc.).
- B. Funding We consider this to be top-priority basic research that should be supported by organizations like NSF, USGS, etc. However, the data and models that result should be of use in solving facies-related reservoir problems in the oil industry. This problem-solving connection should be stressed in designing the projects to encourage joint industry-agency funding for this work.
- C. Clastic Example The Mississippi delta is a site of active modern sedimentation and has a detailed and well controlled stratigraphic framework. The Holocene section there seems to us a good place to begin a new generation of quantitative stratigraphic studies. In addition to the general types of data outlined above we would need:
 - 1. permeability of cored sediments
 - 2. dimensions of facies tracts and individual beds
 - 3. dimensions, grain sizes and orientations of preserved sedimentary structures
 - 4. flow measurements: velocity structure, grain size, bed forms, sediment concentration during floods and major storms, over several years.
- D. Carbonate Example For hydrocarbon accumulation and reservoir studies mixed carbonate/evaporite, mixed carbonate/clastic environments and carbonate build ups are of major importance. We suggest renewed effort at classic sites at Abu Dhabi and/or Belize. Stratigraphic methods would include:
 - 1. permeability of cored sediments

2. dimensions of facies tracts and individual beds
 3. dimensions, grain sizes and orientations of preserved sedimentary structures
 4. flow measurements: velocity structure, grain size, bed forms, sediment concentration during floods and major storms, over several years.
 5. geochemical, emphasizing pore-water and sediment geochemistry.
- III. Clearing house for stratigraphic data

We strongly support the idea of a central clearinghouse for quantitative stratigraphic data. We do not support the idea of starting a new journal or of associating the data base with a journal. It is not possible at this point to specify which data should be collected, and we expect the material stored would include both paper and electronic data. We recommend the USGS, or the Texas Bureau of Economic Geology as possible library and storage sites. In addition, journals should be encouraged to publish detailed stratigraphic data suitable for model testing.

REPORT OF WORKING GROUP 4 (2/18/88)

Future Directions in Confirming and Refining QDS Models with Stratigraphic Information

Group Members: Matt Matthews (Moderator), Ashton Embry, Benito Guerrero, Warren Huff, Terry Quinn, Bill Ross, Keith Shanley, Rudy Slingerland, Michael Steckler, James Syvitski, Dave Valasek

1. Testing depends on who the customer is, what they are trying to achieve, what the critical results are, and what is necessary to predict it. What we attempt and use to verify the model depends on that.
2. Depositional unit scale (short time frame).
 - A. Time stratigraphy (next 5 years).
 - 1) 5,000 years, Milankovitch cycles.
 - 2) Throughout the unit of interest and into bounding units.
 - 3) Sampling should concentrate on boundaries as well as the potential for nonlinearity in the unit of interest.
 - 4) chemical dating should be aware of what is being analyzed rather than a bulk mixed origin sample.
 - B. Time stratigraphy (5-10 years).
 - 1) Resolution should be sufficient to recognize duration of transitions and at least 3 points within unit of interest to check for variable depositional rate.
 - 2) Sampling and resolution sufficient to avoid aliasing.
 - C. Lithologic stratigraphy
 - 1) Standard microstratigraphic techniques.
 - 2) Directional permeability (3 orthogonal directions), x-radiographs at oriented core for internal structures, thin sections, 3 orthogonal directions.
 - D. A good understanding at averaging, preservation, and identification of deposited material is needed in order to extend engineering scale studies in this scale.
 - E. Recommend a detailed study of a 1 million year stratigraphic sequence in a series of staged experiments.
 - 1) Start with definition of the area of interest
 - a. position of globe, boundary conditions.
 - b. predict gross distributions of environments, seismic reflectors.
 - 2) Add depth ranging geophysics
 - a) Data-seismic, MT, EP, TM, gravity, magnetics, etc.
 - b) evaluate previous predictions.
 - c) predict geometry of major interfaces and gross character of units (size, shape, thickness, grain size, mineralogy, porosity, permeability).
 - 3) Add a few oriented cores.
 - a) Data microstratigraphy, etc.
 - b) evaluate previous predictions.
 - c) predict depositional facies, size, shape, thickness, grain size, sorting, mineralogy, porosity, permeability, etc.
 - 4) Final detailed oriented coring program.
 - a) Data microstratigraphy etc. locations chosen to evaluate predictions from #3.
 - b) evaluate previous predictions (diagenesis, pore waters, bedding etc.)

- F. Create an ocean drilling program to gather oriented cores in shallow (less than 400m) water including borehole logging and imaging.
- G. Identify existing data and utilize it with new QDS perspectives.
- 3. Engineering scale, real time.
 - A. Time stratigraphy - wall clock.
 - B. Establish boundary conditions.
 - 1) Before
 - 2) After
 - 3) Edges
 - C. Measurements during.
 - 1) Energy conditions (time and space)
 - 2) Transported sediment
 - 3) Deposited sediment
 - 4) Remobilization
 - 5) Erosion
- 4. Exploit the present.
 - A. Establish what models exist, what they are supposed to do and their assumptions or limitations.
 - B. Establish existing data bases.
 - C. Create from existing or new efforts at least 3 different data sets for each stratigraphic condition.
 - D. Use these reference data sets to test models against both for accuracy and portability.

REPORT OF WORKING GROUP 5 (2/18/88)

Interdisciplinary Applications of QDS Models and their Requirements

Group Members: Tony Gorody (Moderator), Souad Al Azzawi, Stefan Bachu, John Barwis, Frank Caruccio, Mark Chapin, Shirley Dutton, Peter Flemings, Dennis Kolata, Laird Little, Didier Masson

Interdisciplinary approaches are based on the need to improve our understanding of the rock fabric/framework, fluid flow, and rock-fluid interaction. Any and all disciplines that can impact this goal need to be included.

To define its role towards the realization of this goal, each discipline must first address specific problems and decide upon model requirements to solve the problems. Multiple model concepts (hierarchy), could be required that may or may not incorporate QDS techniques in a complementary fashion.

Some debate revolved around the issue of defining QDS and its role in supporting interdisciplinary problem-solving needs. There were a wide variety of perceptions suggesting that QDS comprises:

1. techniques to facilitate geologic interpretation through data acquisition, automated data processing, and graphics output;
2. any type of simulation or model that uses mathematical and physical principles to quantify dynamic geologic processes;
3. any quantitative approach that predicts temporal and spatial distribution of sediments at any appropriate scale, resulting from the simulation of the genetic process.
4. any quantitative approach that allows an earth scientist to test hypotheses by interacting with a computer terminal at a speed that won't interrupt a train of thought.

Potential Applications

The participants in the workshop had numerous interests and represented many disciplines. They felt that QDS techniques could be applied to many of their needs. Their "wish lists" provide a glimpse of the many potential application for QDS. These include:

- A. Hydrocarbon exploration
 1. predict spatial geometry of depositional systems at all scales and determine where reservoirs and source rocks occur; calibrate with modern analogs whenever possible.
 2. Predict spatial distribution, volume, and composition of source rock facies
 3. facilitate data integration among well logs, seismic sections, outcrops, core, and cuttings analysis.
- B. Minerals exploration
 1. predict mega-scale fluid flow, the distribution of dissolved chemical species, and sites for mineral precipitation

2. visualize spatial evolution of permeability
- C. Geotechnical applications:
 1. improve siting criteria on the basis of improved knowledge regarding the interdependence between lithologies and their geomechanical, physical properties
 2. improve planning to conduct preliminary investigations for design purposes
- D. Reservoir engineering and production:
 1. predict behavior of multiple phase fluid flow with time as reservoir is produced;
 2. optimize pressure maintenance strategies;
 3. facilitate planning for and maximize recovery from injection and production wells for secondary and tertiary recovery schemes;
 4. develop quantitative relationship between production profiles and evolution of reservoir dynamics during production;
 5. quantitatively integrate reservoir engineering models with geologic facies models;
- E. Development drilling and field extension:
 1. predict grain size distribution, porosity, sand body geometries, permeability distribution, and degree of interconnectedness between permeable sedimentary packages;
 2. re-interpret stratigraphic relationships using new methods to evaluate old data, and refine correlation techniques;
 3. predict the distribution of litho-hydraulic units and their relationship to primary depositional architecture and subsequent diagenesis;
 4. provide reliable models that include the effects of fracture flow in addition to matrix permeability;
 5. model single and multiple phase fluid flow through depositional systems;
 6. improve infill drilling strategies by optimizing well density and spacing geometry;
- F. Sedimentology and stratigraphy
 1. provide an accurate time-stratigraphic framework of sediments in a basin and identify third and fourth order sequences.
 2. improve our understanding of the genetic relationship between facies migration and tectonic/eustatic effects ;
 3. Generate new insights on stratigraphic concepts such as: under what condition does ravinement occur?; likely scenario for fluvial aggradation;
 4. provide a quantitative basis for improved inter and intra-basinal correlations.
- G. Diagenesis:
 1. provide models that predict fluid flow rates in various geologic settings as a function of topography, stratigraphy (sand/shale ratio), and permeability as diagenetic modification occurs;
 2. eventually combine fluid flow models with fluid-rock interaction models;
 3. predict geothermal gradient through time in sedimentary formations (or heat flow), during hydrocarbon generation, expulsion, migration, and accumulation, and determine the influence of sedimentary basin fluid flow on the geothermal gradient;
 4. reconstruct pathways for hydrocarbon migration and resolve lateral and vertical migration components;
 5. in all cases provide user friendly models so that the geologist can concentrate more on solving geologic problems than on solving programming efforts.
 6. model multiple phase fluid flow (gas, oil, and water) to re-examine specific issues such as: can water flow through oil-filled rocks?; does diagenesis continue after oil has entered a reservoir?;
- H. Coastal Engineering
 1. predict coastal sediment transport and change in transport properties with time to improve design and siting of coastal structures;
- I. Hazardous waste disposal:
 1. Improve deep disposal models to optimize injectability, better determine fracture threshold, predict the spatial distribution of hydraulic properties;
- J. Risk Analysis
 1. provide interactive QDS models that interface with increasingly sophisticated economic models, ROR, etc., to better guide management decisions and provide tools for sensitivity analysis
- K. Modeling
 1. Turning the problem around by obtaining verification of input parameters that bear on paleoclimatology (prevailing winds, oceanic circulation patterns), paleobathymetry, paleogeography (paleo shoreline position), paleosalinity, paleotemperature, i.e. a reliable data base with which to calibrate models.

Status

Most of the workshop participants felt that although QDS techniques appear to be at a relatively young stage of development, the potential for growth was excellent. There were some major problems that were identified to be currently influencing the growth rate. For example, adequate quantitative data bases that can help verify QDS models are limited. The kinds of measurements required for this new discipline often have not been made, and those data that are available, are for the most part crude, lacking in standardization and consistency. Once this problem is improved, QDS techniques should advance greatly.

Another problem identified is that investigators who could benefit from existing models are not using them because they may not be aware that they exist. Such models were developed to solve other problems outside of their own particular disciplines. The availability of models among disciplines are also in varying states of evolution and can be difficult to adapt. Therefore seemingly independent disciplines need to coordinate their efforts along these lines before interdisciplinary approaches can be fully successful.

Yet another problem lies in the differences in the level of accuracy which are required when modeling at different scales. For example, fairly realistic and advanced models are available on small temporal and spatial scales. This is especially the case when relatively few, but well understood, mathematically described physical principles are used to constrain the models. However, models which examine complex and large systems, are more poorly understood and require huge simplifying assumptions about the way processes work. For them to more adequately approach physical reality, they have to be precisely calibrated to an adequate, numerical data base. Trial and error, continued interactive hypothesis testing, and increased confidence in the results obtained from adequately constrained models, will also be required for improvement. This is likely to be an evolutionary process.

In some respects, currently available QDS models are competing with genetic stratigraphic approaches. Each can provide the framework by which interdisciplinary problems can be attacked. However, for QDS to be more fully accepted, the perception that such techniques must mirror reality needs to be dispelled. It should be replaced with the perception that QDS provides a quantitative framework with which to simulate reality, thereby providing a means to test hypotheses, and gain insight on processes that are not intuitively obvious. The experience gained by those already active in this field has also demonstrated that the process of quantification (numeric representation) alone can be helpful in bringing out interrelationships that otherwise would have remained obscure.

In spite of the apparent drawbacks currently being encountered, the probability of success for integrating workable models and understanding their interdependency within next 5-10 years is great. This will require close interdisciplinary cooperation and carefully coordinated funding.

Recommendations

We would like to invoke the "man on the moon" analogy for focusing what is currently a widely diverse and diffuse effort. As forecast at the time of the announcement, it took one decade to place a man on the moon. That goal was achieved as a result of an intense interdisciplinary effort which was well managed and well funded. The spin-offs from that project, somewhat unexpected, also heralded the age of miniaturization and the computer age.

In this context, it would be wise to attack a specific and challenging problem of national importance which would lend itself to the convergence of an interdisciplinary effort. The evolution of QDS techniques could provide the tools required to solve such a problem. For example, many of us have shared our concerns at this gathering over the increasingly serious problem of groundwater contamination. What if we decided to tackle the Dakota aquifer system using a quantitative dynamic stratigraphic approach? This aquifer system has all the elements required to address most of the applications suggested by this panel. It encompasses a variety of depositional systems, it transmits water, oil, and gas, it is contaminated in places, it resides in an area where water is relatively scarce, and a large data base is available that has just recently been compiled and published. Within the context of such a program, there could be many other objectives. For example

QDS could predict the spatial distribution of sand, silt, clay layers in order to assess the flow and directional velocities of low density and high density non-aqueous liquids (NAPL's).

In order to realize such an effort, we envision the organization of a national center of excellence for this purpose. The center could be devoted to pure research, an RFP could be issued soliciting innovative ideas, and various consortia for applied research could be dedicated to supporting such an effort. We envision that this should be a multimillion dollar effort, funded by private and public concerns and including local, state, and federal government.

REPORT OF WORKING GROUP 6 (2/18/88)

Integration, implementation, and transfer of QDS models

Group Members: Klaus Bitzer, Marc Ericksen, Mike Gardner, Ray Gildner, Gigi Grace, Chuck Norris, Van Price, Fred Schroeder, Will Schweller, Dan Tetzlaff, Michael Zeitlin

Introduction

Group six was charged with the question of how to improve communication among modelers and among programs. We subdivided our tasks into three categories: Communication and access to models; Computer guidelines for portability enhancement; and Categorization of model types.

Communication and access to models

Certain organizational elements are essential to inform the geoscience community and expedite communications among model builders and model users. These elements should be set up in a chronological order:

- A long-term organization is necessary to set up and maintain the communication system.
- An Electronic Bulletin Board should be set up to facilitate rapid communication such as requests for information or announcements of available programs and databases.
- A Georef database should be set up to classify publications on modeling in terms of parameters defined from the survey.
- Formal announcements of the Electronic Bulletin Board, the Georef database, and the central organization should be published in as many journals and newsletters as possible. Places include Geotimes, EOS, AAPG Explorer, SEPM newsletter, GSA News and Information, GEOBYTE, etc.
- A QDS Newsletter should be established for international communications and for general announcements to those who do not access electronic networks.

Computer guidelines for portability enhancement

Model development using computers is usually done by the modeler/ programmer in such a way as to achieve the goals in the shortest possible time. Little concern is given by the modeler that somebody other than the authors might use the code. Some guidelines are offered, therefore, that are intended to maintain the creativity and productivity of the modeler, while allowing for easier transfer of models to other users and the integration with other models. We believe guidelines would be useful in the following three areas: program languages, operating systems, and code structure.

Programming Languages

The following two languages should be used whenever possible: Fortran - for numerical computations, and "C" - for graphics and symbolic manipulations, including Artificial Intelligence applications. This recommendation is based upon the appropriateness of these languages to problems commonly encountered in QDS, and their availability for the next five years. Fortran is recommended because of its continuing widespread use and existing library of code. "C", although less well known, is rapidly growing in use and support, and facilitates process to process communications. "C" is well suited to bridge to the protocols of the future. Where other languages are used, the code should be particularly well documented to enable easier portability via translating, or compilation into compatible object code.

Operating Systems

The following table shows operating systems commonly in use in each computing environment. Networking, portability, data transfer, and model implementation are all enhanced by a common operating system protocol. Unix is the only operating system that can easily be implemented, independent of vendor, in these categories. It is powerful and flexible for all levels of users.

Personal Computers	Workstations	Mainframes and Supercomputers
MS-DOS	DEC/VMS	DEC/VMS
OS2	UNIX	UNIX
UNIX shells	VM-CMS	COS
Macintosh		NOS-SCOPE2
		MVS

Code Structure

Code should be modular. The three fundamental structural components are: graphics (including input and output); numerical calculations; and, database. As a minimum, any code should be structured to reflect these three logical components. This can be done by writing self-contained routines that can be called by a master program or other subroutines. Within each of these components, code should be further broken into logical functional subroutines. Each module in this hierarchy should be fully documented with respect to function, reference, input variables, output variables and special considerations.

Categorization of models

Describing models in terms of their subject, scales and parameters is a useful way to facilitate communication among QDSers. Attendees at the Workshop were surveyed as a test of a preliminary categorization scheme. A copy of the survey form is attached as an appendix. The following topics were included:

- Type of model
- Approach
- Primary objective
- Processes/Input
- Boundary conditions
- Output displays
- Computer requirements
- Numeric and Graphic languages
- Mathematical rigor
- Status

Results of the survey are presented below as a series of pie-charts.

MODEL INVENTORY FORM

Program Name: _____

Institution: _____

Contact: _____

Phone: _____

Address: _____

Date Developed: _____

CLASSIFICATION: (Prioritize as applicable)

Type: Conceptual___ Empirical___ Stochastic___ Analytical___ Heuristical___ Other___

Approach: Forward___ Inverse___ Mixed___

Spatial Dimensions: 1-D___ 2-D___ 3-D___

Temporal Scale: Minumum___ Maximum___

Typical Model Dimensions: ___(x)cell ___(y)cell ___(z)cell

Fundamental building block modeled:

Sediment particles:___ Facies:___ Sequences:___ Other___

Primary Objective:

Stratigraphic___ Fluid Dynamics___ Thermal/Maturation___ Rock Properties___

(Correlations/facies)

(flow networks)

(Heat flow, TTI)

(porosity/permeability)

DESCRIPTION:

(circle as many as appropriate)

Processes/Input

(c= constant in time, v= variable in time, D= dynamic, circle one)

weathering C V D

transport C V D

surface flow C V D

compaction C V D

erosion C V D

deposition C V D

subsurface flow C V D

Sed. quantity C V D

topography C V D

-non-marine C V D

eustacy C V D

Sed. type C V D

climate C V D

-mar./clastic C V D

paleobathymetry C V D

Isostatic Comp. C V D

lithosphere C V D

-carbonate C V D

porosity C V D

diffusion factor C V D

permeability C V D

tides C V D

waves C V D

oceanic circulation C V D

Others_____

Boundary Conditions:

Output Parameters:

Models observe conservation of: Mass___ Momentum___ Energy___ Space___

Output Displays: Columns___ Cross-sections___ Grids___

Time vs Depth___ Maps___ Perspectives___ Others___

Computer:

Super___

Mainframe___

Workstation___

PC___(type)

Memory requirements:

Modules:

Database:

type_____

public (Y/N)

Numerics:

how handled_____

Language_____

Graphics:

Language_____

Overall mathematical rigor: 1 2 3 4 5 6 7 8 9 10

(circle one)

basic

rigorous

Status:

(circle one)

1 2 3 4 5 6 7 8 9 10

prototype

released

Model Types

Dimensions

Approaches

Output

Model Constraints

Computer Type

Language

Graphics Languages

REPORT OF WORKING GROUP 7 (2/18/88)

Potential Impact of QDS on education, science, engineering, and public policy

Group Members: Harry A. Tourtelot (Moderator), Charles Gilbert, Roice Nelson, Marty Perlmutter, Chris Shaw, Tonya Thorn Dyce

This topic focuses on matters external to the QDS community, and thus differs from those of other working groups whose assignments deal more with QDS subject matter and procedures. The entities to be impacted by this Working Group are nebulous targets without clearly seen points of attack. The results of our deliberations similarly lack precise form and focus.

Rather than answer each question as presented to us, we have decided to speak to two general topics extracted from the questions, acceptance of QDS and cost benefits, and then the impacts of QDS on education, science, engineering, and public policy.

Acceptance of QDS

Fundamentally, QDS will be accepted in almost direct proportion to the extent that it is perceived to be useful by whatever audience is potentially concerned. Some general points of resistance can be recognized, however, such as lack of understanding, physic distrust of numerical approaches by nonmathematical people, belief that numerical models oversimplify, and classic conservatism based on a dogmatic orientation. People who resist for these reasons, and no doubt others, are found in all levels of industrial management, academic circles, government, and within the QDS community itself.

This kind of resistance can be overcome. Fundamentally, a strengthened training base in quantitative geologic approaches should be employed at the undergraduate level, so that the mathematical "blind spot" no longer exists in degreed geologists. In dealing with geologists already in today's work force, an increased level of exposure to the basic premises and successful usage of QDS would inform the geologic public that the stratigraphy is evolving into a more quantitative discipline. This exposure could be effectively delivered through publication in the widely read geologic journals and newsletters of the major geo-organizations. To prove the value of QDS, old things will have to be done better (more reliably, cheaper, faster). New kinds of things to be done will inevitably appear, as concepts and techniques continue to develop, so that problems that were formerly (pre-QDS) unassailable can be tackled. Individuals will have to define the roles that QDS can fill in scientific research, in resource discovery and exploitation, and build case studies of successful applications and relations to other quantitatively oriented geologic subdisciplines. Individuals should focus effort on problems that matter and publish in widely read journals as well as those of specialties.

Cost benefits, risks, and economics

This is a very diffuse subject that hardly can be considered without reference to specific activities. The only thing about cost benefits that stands out clearly is that there better be some. If QDS cannot do something better, cheaper, faster, and therefore have positive cost benefits, then perhaps its ways should be changed. The risks associated with QDS, like those attached to any activity ranging from resource exploration to writing a paper, have to be taken by individuals not special interest groups. The economics of QDS depends on the subject and the potential funding sources around the subject. The economics in this context depends on QDS building a better mousetrap.

Impacts on education

The successful practice of QDS demands workable skills in mathematics at advanced levels. This is merely the present state of a historical trend of increasing quantification in science, a phenomenon that began in geology about 30 years ago. To construct better models we need to build better modelers. Education thus impacts QDS more than QDS impacts education in the broad sense.

In addition to mathematics, QDS integrates many, if not all, geologic fields and makes obvious the need for more rigorous training in a wide range of branches of the earth sciences, computer skills and modeling philosophy. Geology departments may need to deal themselves with courses in ancillary subjects (i.e. mathematic and computer applications) to maintain a geologic context for research and application.

Impacts on science

It is assumed that this means earth science: nuclear physicists are not likely to be impressed by what we do. The most significant impact is that the use of quantitative methods will grow. This will lead to the more intensive and effective investigation of larger and larger areas with the ultimate effect of making it possible to examine global processes.

Impacts on engineering

If the abilities of QDS continue to grow and more real world problems are tackled, the impact on engineering is likely to be pretty much of a jolt. Many engineering activities such as waste disposal or contamination clean up can be approached effectively only by large applications of QDS techniques. Other societal problems requiring large models and on which QDS should have an impact include analysis and exploitation of water resources, energy resources, and mineral resources. The engineering community will continue to apply methods of the past to these problems until QDS can demonstrate that this kind of quantitative approach is what is needed for engineers to develop better solutions. We need intelligent linkage with the engineering community. Activities such as those at the Savannah River Plant could be a very effective opening wedge.

Impact on public policy

Public policy is hard to change. In general, public policy demands solution of problems without being much concerned with methods. Policy is made by people, and that is whom we have to impact. The difficulties of this are an integral part of the general problem of increasing the understanding of science by the general public as well as people at high levels in government. If QDS work is effective, the situation might improve, but it no doubt would do so slowly.

Where the geological problem requires it, project plans and proposals should not be limited by political boundaries. The regional nature of the work should always be emphasized, if it is at a regional scale, and this could lead to less localized and chauvinistic political responses.

Final comment

QDS is an exciting development of powerful techniques for attacking major earth science problems of increasing societal concern. These developments have to continue with great emphasis on the research mode. At the same time, if QDS is to win the acceptance and play the important role we all hope for it, opportunities are going to have to be sought to demonstrate that QDS is in fact a better mousetrap.

END

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