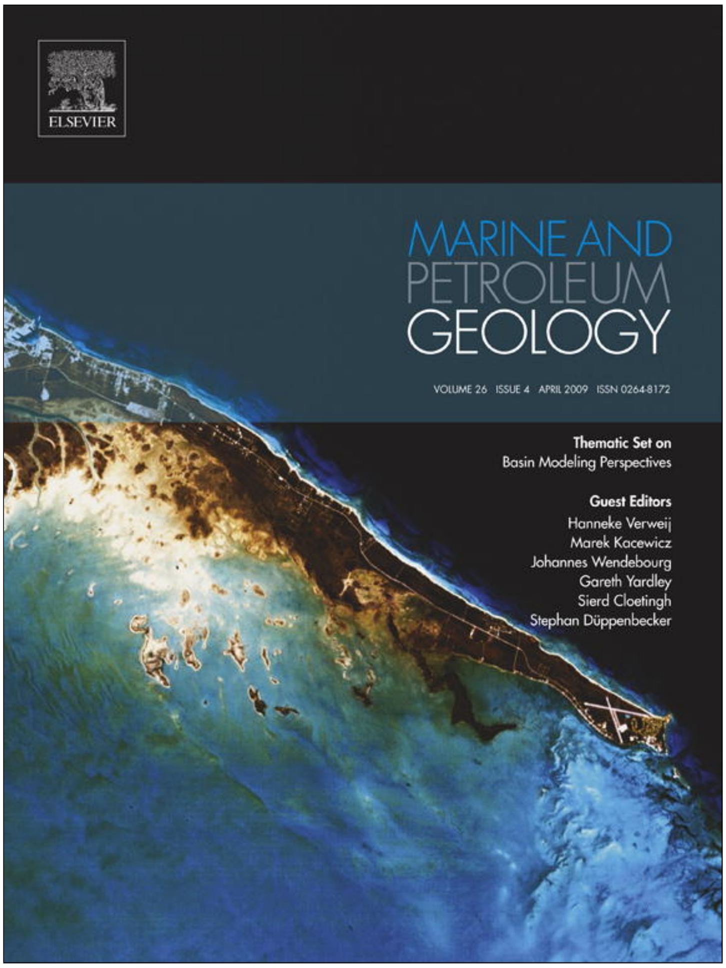
ELSEVIER
MARINE AND PETROLEUM GEOLOGY
VOLUME 26 ISSUE 4 APRIL 2009 ISSN 0264-8172
Thematic Set on
Basin Modeling Perspectives
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Marine and Petroleum Geology 26 (2009) 487–494

Contents lists available at ScienceDirect

Marine and Petroleum Geology

journal homepage: www.elsevier.com/locate/marpetgeo

The potential benefits to the basin modeling enterprise of modularization and incorporating organic and inorganic chemical change

L.M. Cathles*

Earth and Atmospheric sciences, 2134 Snee Hall, Cornell University, Ithaca, NY 14853, United States

ARTICLE INFO

Article history:
Received 13 September 2007
Received in revised form
16 March 2008
Accepted 2 January 2009
Available online 15 January 2009

Keywords:
Basin modeling
Chemistry
Alteration
Carbon dioxide
Gas washing
Dynamic link libraries (DLLs)
Modeling strategy

ABSTRACT

Mineral and hydrocarbon resources in basins are produced by fluid movements whose nature is not fully understood. Flow models in realistically defined basins that predict chemical change are needed to make progress, but these models will be difficult to develop and keep vital. Two simple examples are given to illustrate what is required, and the challenges to basin modeling are then outlined. It is argued that the best strategy is to modularize existing physical and chemical codes and place as many of these modules as possible in the public domain. This will keep the modeling enterprise open to the new entry and continuing invigoration.

1. Introduction

The purpose of this paper is to suggest that we should actively seek to incorporate inorganic and organic chemical change into basin models. The potential value of such incorporation is illustrated with two, recently published, examples. A further objective is to suggest that the vigor of the basin modeling enterprise can be maintained if, and perhaps only if, we adopt a strategy of component or interchangeable module development.

In the simplest terms, chemical change should be incorporated into basin models because it records the past movements of basin pore fluids. Since the movement of pore fluids produces both hydrocarbon and mineral resources, clear knowledge of it is a foundation of effective exploration. One might think we would already know all there is to know about fluid movements in basins, but one only needs to list the very different views of fluid movements through faults (directly up dilation paths within the fault, in the faults but only when the fault is moving, in the fault but only when appropriately overpressured, only in the damage zones around faults, never through the fault but by crossing the fault to step up stratigraphically where sands are juxtaposed) and the host of issues surrounding the impact of capillarity on fluid flow, to realize that this is not the case. It is convenient that the resources we seek are themselves chemical anomalies, and therefore the needed chemical samples are largely already collected. But the essential point is that the past movement of fluids is written exclusively in chemical change, and therefore to understand fluid movements we must develop models that predict the chemical changes that are caused by fluid movements.

Two examples illustrate how incorporating chemical change into basin models might help. The first shows how chemical changes that are associated with gas washing (the alteration of oil by its interaction with migrating gas) might, if suitably modeled, provide a means to investigate how hydrocarbons have utilized faults in their migration. The second shows how models of the migration of CO_2 generated in deep, hot basins to cooler, shallower environments where it reacts with sediment minerals and crystallizes as carbonate could provide insights into how the migration of CO_2 gas is influenced by faults. These examples illustrate one potential benefit of incorporating chemistry into basin models, but defining the pattern of past fluid movements could, of course, have many other benefits.

Combining complex chemical models with already complex physical basin models is not be a trivial task. The final section considers how this, or any other new development in basin modeling, might best be cultivated in a simulation environment

* Tel.: +1 607 255 2844; fax: +1 607 254 4780.
E-mail address: lmc19@cornell.edu

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doi:10.1016/j.marpetgeo.2009.01.001

that is increasingly dominated by very large and inclusive models that purport to include all "known/important" basin phenomena. The issue considered is how to keep the modeling enterprise fresh while it is, at the same time, becoming increasingly broad and capable. This was the theme of a recent Hedberg Conference on basin modeling, and preparation of a presentation for that conference motivated the thinking recorded here.

2. Two models of chemical change in basins

2.1. Petroleum movements in the offshore Louisiana Gulf of Mexico

Fig. 1 shows some features of a 100 × 200 km Corridor that starts at the Louisiana coastline and ends just past the shelf edge. The Corridor includes the Tiger Shoals oil and gas fields near the coast, the South Eugene Island Block 330 in its middle, and the Jolliet field and the Bush Hill hydrate mound and gas seeps at its southern end. In its middle, the top of overpressure (as depicted by the 12 ppg mud surface) lies 3–4 km below the sea floor as shown in Fig. 2d, but past the southern end of the section the top of overpressure surface almost touches the sea floor. The maximum thickness of the basin sediments along the Corridor is ∼16 km (Fig. 2c).

Fig. 2 shows how today's stratigraphy can be extracted from a published section, and Fig. 3 shows the geologic evolution of the section can be inferred by backstripping and decompaction in a conventional fashion.

Assigning basal heat flow to the geologically evolving section using a rift model, thermal conductivity using a fabric model that includes changing porosity, and radiogenic heat generation according to the sand–shale ratio, it is found that the observed present heat flow, temperature profile, and vitrinite reflectance along the section is matched without any modification of the parameters taken from the literature. The heat flow is depressed by nearly a factor of two by the very rapid recent sedimentation in the middle of the corridor, and increased by nearly 50% by radiogenic heating in the sediments.

The two source strata shown in Fig. 2 mature as the basin grows and the sediments heat. If the oils and gasses generated in these source strata migrate vertically and a 20% saturation of the pore space of the source strata is required for the model petroleum to leave the source strata, the gas saturation in the strata overlying each source must be less than 0.5% for petroleum to vent into the Gulf as observed, and the petroleum saturation must be ∼0.025% for Eocene oils to dominate, as observed, in the northern part of the section (Fig. 4). Very little petroleum is stored in the model subsurface between the source strata and the surface.

Dry gas is sweeping the section today and this gas has altered the chemistry of the oils. Fig. 5 shows the remarkable observed pattern. As articulated first by Meulbroek et al. (1998) for the Eugene Island area, and subsequently extended to the whole transect by Losh et al. (2002) and Losh and Cathles (2002), Fig. 5c shows that, in the northern part of the section, over 90 wt% of the $C_{10}+$ *n*-alkanes have been carried off (and largely vented in to the ocean) by dissolution into a gas phase, whilst none has been so removed in the southern part of the section. The pattern of chemical change is remarkably regular, with just enough irregularity in the middle to be interesting. The pattern is expected. The greater oil alteration in the north results from the greater maturity of and gas generation by the source strata there.

Examining the 138 oil analyses collected by our study in a geographic context within a GoCad data base (Cathles et al.,

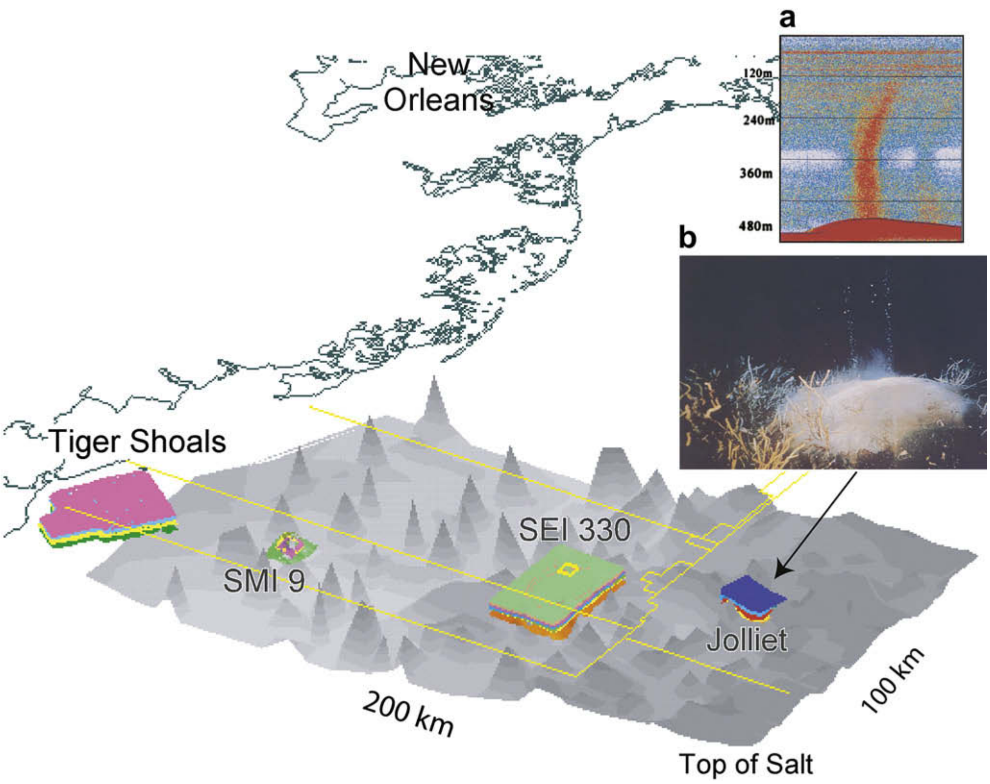

Fig. 1. Location of the 200 km N–S by 100 km E–W GRI Corridor off the Louisiana coast within which we modeled hydrocarbon generation, migration and venting, and the associated organic chemical changes. 3D seismic surveys at Tiger Shoals, South Marsh Island Block 9 (SMI 9), South Eugene Island Block 330 (SEI 330) and the Joliet oil and gas fields are shown. (a) A sonic image of the gas plume emanating from the 800 m diameter Bush Hill mound at a depth of ∼540 m from Sassen et al. (2001). (b) Methane venting from ∼1.5 m diameter hydrate patch of the Bush Hill mound near the Joliet drilling platform photographed by Ian MacDonald.

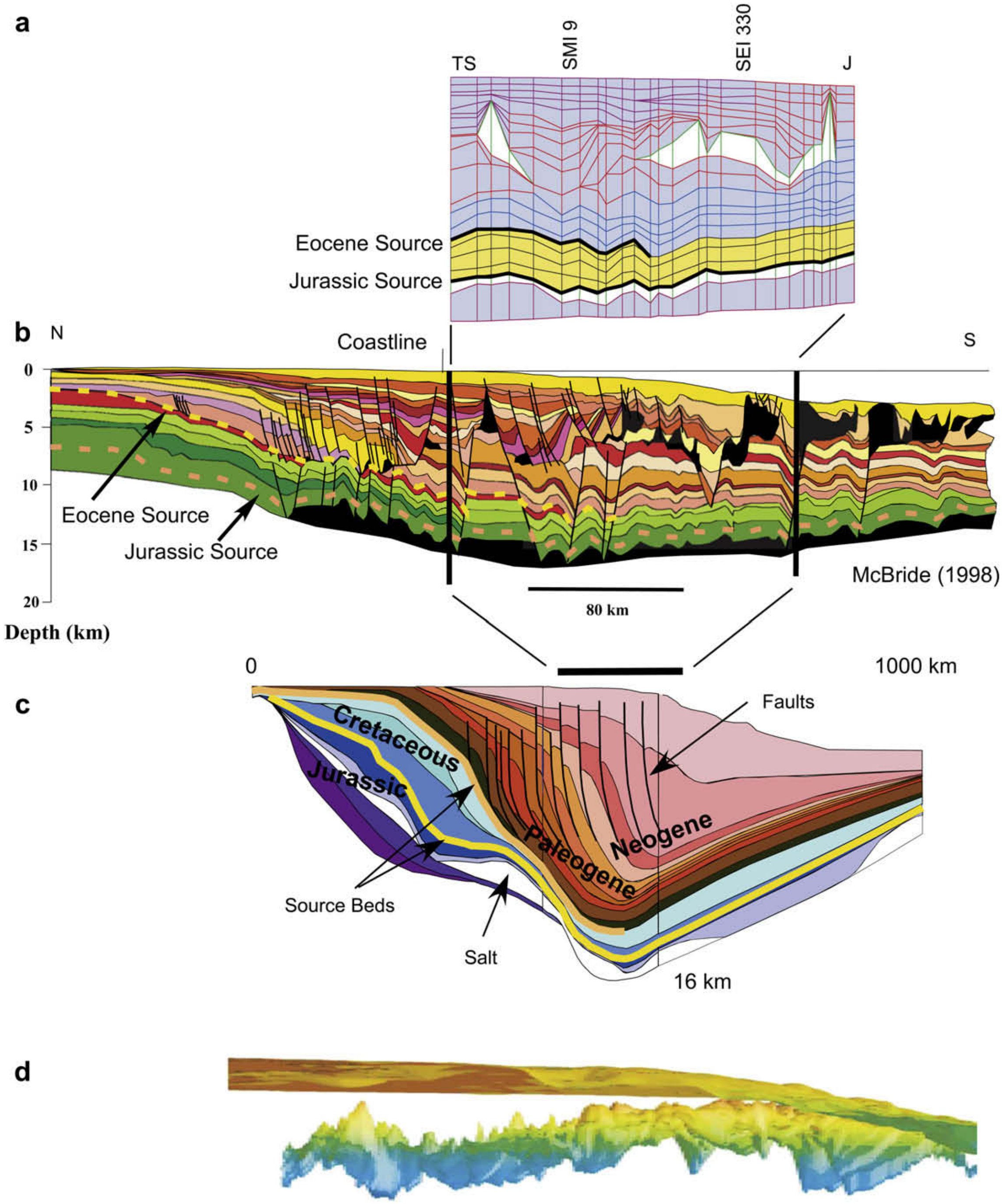

Fig. 2. The subsurface interpretation of a N–S section across the GRI Corridor we model (a) is extracted from a section (b) geologically interpreted by McBride (1998) whose position is also indicated along a 1000 km N–S section (c) that runs from the Louisiana–Arkansas border to the Sigsbee Knolls in the Gulf of Mexico. The top of overpressure (as measured by the 12 ppg mud surface which we extracted from header logs) throughout the Corridor is shown in (d).

2002), the intensity of gas washing can be seen to differ significantly in different sides of the South Marsh Island Block 9 field shown in the northern end of the Corridor in Fig. 1. The oils are washed more intensely on one side of the dome than the other. To be washed more intensely the oils must have been subjected to a stronger, more focused gas stream. A denser grid of petroleum analyses could reveal this gas stream (locus of more intense washing), and modeling of this stream could reveal how faults and stratigraphy control petroleum migration. Adding gas washing to conventional models could thus provide a way to advance our understanding of how fluids move in basins.

An extensive report to the Gas Research Institute (Cathles, 2002; Cathles and Losh, 2002) gives full details of the modeling described above. A number of papers provide shorter summaries (Cathles, 2003, 2004).

2.2. The generation and titration of CO_2 gas in basins

The second example is the generation, migration, and titration of CO_2 gas in sedimentary basins. Modeling details can be found in Cathles and Schoell (2007). Fig. 6 illustrates how CO_2 is generated in a CO_2 kitchen below the much shallower oil and gas kitchens that

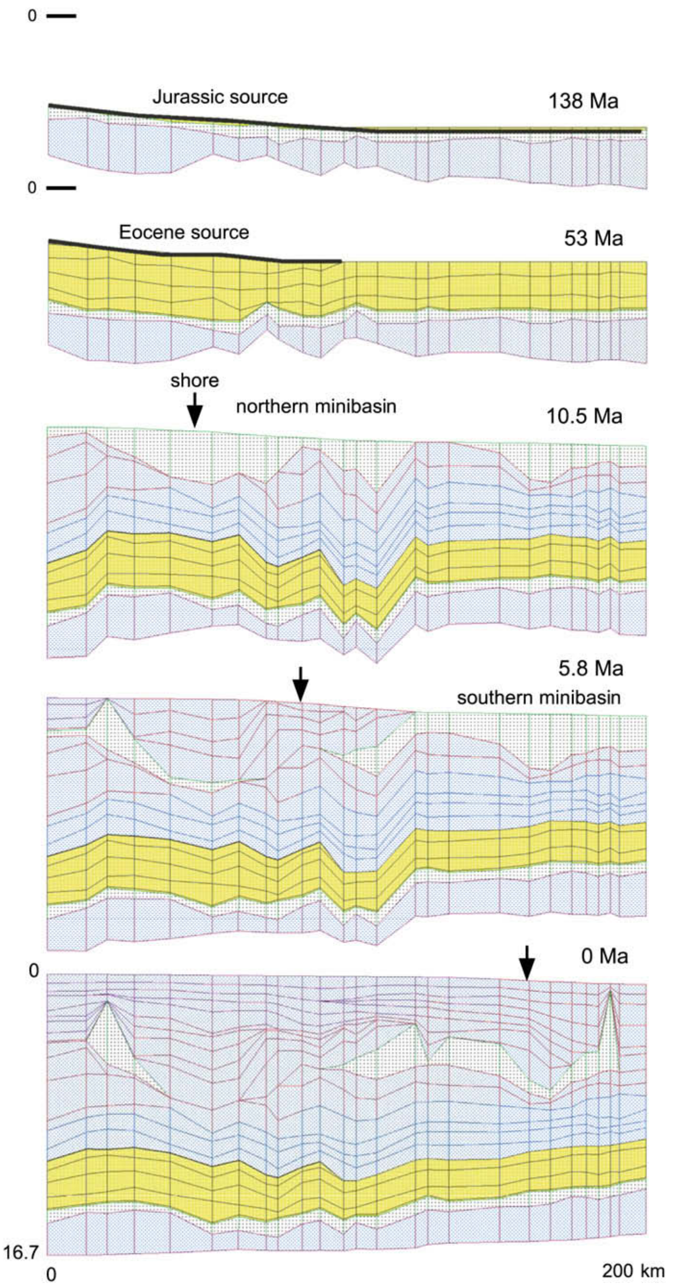

Fig. 3. The evolution of the Fig. 2a section, obtained by backstripping and employing a salt migration algorithm that redistributes salt from areas of higher to lower average rates of sedimentation. Notice that the Louann Salt is capped with the Jurassic source beds at 138 Ma. A carbonate sequence is capped with the Eocene source strata at 53 Ma. Silicate deposition follows. The Louann salt is inverted to a surface sill between 10.6 and 10.5 Ma. The salt in the sill is then remobilized to form salt-withdrawal minibasins as it is loaded by sediments, first in the northern half of the section (to 5.8 Ma) and then in the southern half. The end result is the present stratigraphy along the section.

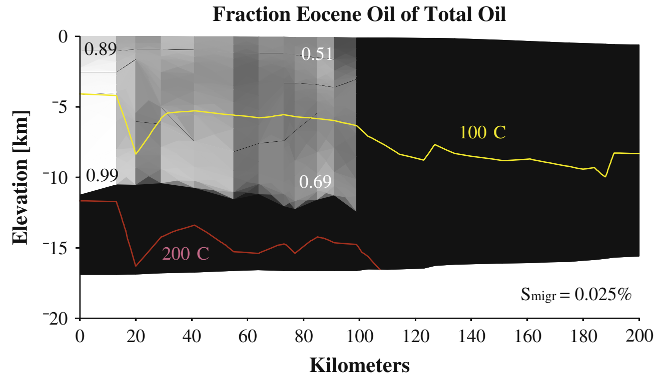

Fig. 4. The present-day mass fraction of Eocene to total oil computed assuming a migration saturation of 0.025%. Later-generated Eocene oils dominate the petroleum chemistry above the Eocene source strata. The hydrocarbon flux was computed from the thermal history. The 100 m thick, 5 wt% TOC, type II Jurassic source shown in Fig. 2a was matured using a standard Burnham and Sweeney Type II model. The 30 m thick, 4 wt% TOC, Type III Eocene source strata shown in Fig. 2a was matured using a Wilcox coal Rock-Eval pyrolysis compositional kinetic model contributed by industry with CO_2 generation and oil cracking added.

are the subject of conventional basin models. When basin temperatures exceed ~320 °C, clay formation can combine with acid neutralization by carbonates to produce a separate CO_2-rich gas phase. The key is phase separation because once CO_2 can escape into a gas phase that migrates out of the reaction zone, the concentration of CO_2 in the aqueous pore fluids can no longer increase to the levels required to stop the reaction. When the partial pressure of CO_2 and steam exceeds the hydrostatic pressure of the pore waters, a fizz-bottle reaction is initiated in which alumino-silicates are hydrated to clays and the acid produced reacts with carbonates to produce CO_2. As carbonate-bearing sediments move through the 320 °C isotherm of a basin, clay is produced, carbonate destroyed, and CO_2 gas expelled into the overlying strata in a process very similar to the generation, expulsion, and migration of oil and gas from the shallower oil and gas windows or “kitchens”.

In this case of CO_2 this is not the end of the story because CO_2 is a highly reactive gas and it will react with calcium-, magnesium-, and iron-bearing alumino-silicates at cooler temperatures higher in the stratigraphy to precipitate the CO_2 as calcite, magnesite, or siderite (the carbonates of Ca, Mg, and Fe respectively). So long as Ca-alumino-silicates are available the CO_2 is titrated to very low partial pressures, and no appreciable CO_2 can fill gas reservoirs. While Fe- and Mg-alumino-silicates are available CO_2 is removed such that, depending on reservoir temperature, CO_2 gas might constitute up to 10% of the charge but not more. If Ca-, Fe-, and Mg-alumino-silicates have all been titrated, a reservoir could fill with 100% CO_2 gas as is observed in some locations. Figs. 7–9 show how a model of CO_2 generation, migration, and titration can be constructed and added to a basin model. In Figs. 8 and 9 the white zones have been titrated of alumino-silicates capable of precipitating carbonate, and the risk of encountering gases with very high mole fractions of CO_2 is very high.

Models of CO_2 generation, migration and titration could clearly be of interest in managing CO_2 risk in gas exploration, but they could also be of value in forensically determining how gases migrate in faulted sedimentary basins. The variation in the mole fraction of CO_2 fill in reservoirs near a localized CO_2 kitchen in a basin, and the relationship of these reservoirs to faults, should reflect to how CO_2 migration is affected by faults, and construction of 3D models of CO_2 generation, migration, and titration could allow this kind of data to be analyzed to understand this influence.

3. Strategic considerations

The two examples just discussed illustrate how incorporating models of chemical change into conventional basin models could allow us to advance our understanding of the flow of liquids and gases in faults – a knowledge that is fundamental to exploring for basin resources. There remains the question of how such incorporation might best be accomplished, and this is part of a broader

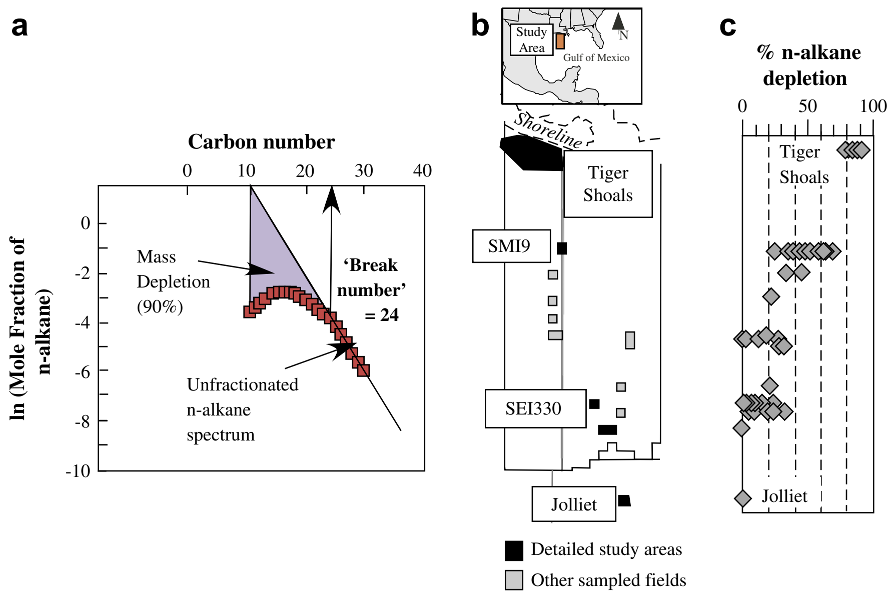

Fig. 5. (a) The removal of low carbon number *n*-alkanes computed when dry gas washes oil can exceed 90 wt% of the $C_{10}+$ *n*-alkane mass. The break number indicates the heaviest carbon number removed by washing. It can be related to the depth at which the washing took place. Sampling locations along the Corridor are shown in (b). (c) Shows there are very regular changes in the pattern of gas washing from north to south along the Corridor.

question of how innovations of all kinds might be facilitated in the future. As one who has personally built, from scratch, a conventional basin model, and also has tried in numerous ways to incorporate chemical and capillary phenomena into such models, I have a personal appreciation of some of the issues involved.

At present the basin modeling profession has two complimentary kinds of models. Some characteristics of these models are indicated in Table 1. One kind of model is what might be called an investigation model, and the other a production model. One person typically builds the investigation model for a specific purpose. It is fully comprehended by that individual but never fully documented and, for this reason, as well as it not being broadly tested or debugged for general application, it is not user-friendly. It is, however, flexible in the sense it is easy to modify, and it is scientifically fertile. It is designed to investigate and test new ideas, and it typically generates numerous publications. Its purpose is scientific and it should, and usually does, allow access to all variables involved in process being modeled.

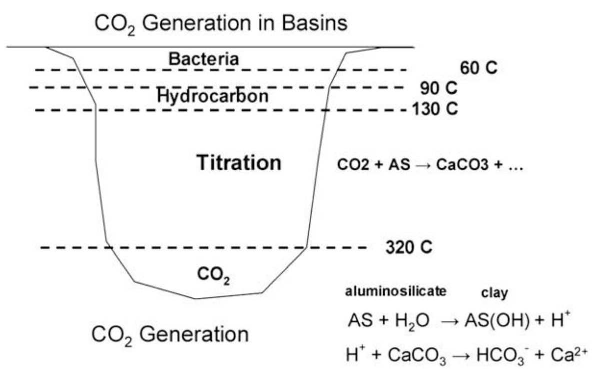

Fig. 6. CO_2 is generated by decomposition of carbonates in sediments as they are buried and heated above ~320 °C. Hydration of alumino-silicates to produce clay generates acid, which reacts with carbonate minerals to produce CO_2. At 320 °C the partial pressure of steam plus CO_2 is high enough for a gas phase to separate. Migrating upward to cooler environments, the CO_2 in this gas reacts with Ca, Fe and Mg bearing alumino-silicates and the CO_2 is crystallized as carbonate. The CO_2 generation and migration is similar to the CH_4 generation and migration that occurs in the gas window as sediments are heated above ~120 °C.

The production model, on the other hand, is built by a group to carry out, in a user-friendly and robust fashion, simulations that are considered useful in exploration or basin evaluation. It is fully documented but there is usually a lot hidden or omitted from the documentation (e.g., scientific details, modeling assumptions, coding tricks, etc.). It is broadly applicable to many basin issues, but can incorporate new processes only with the substantial efforts of the group that maintains the program. Its output is presented in standard form to aid comprehension. Distracting details are not presented and may not be easily accessible. A production model is very useful, but ultimately, to the extent it successfully captures all the important phenomena, it is scientifically sterile. There would be nothing of significance left to discover or discuss.

The two kinds of models are mutually complimentary. Investigation modeling pilots ideas that can be eventually incorporated into production models, and trains scientists that may be hired to further develop or to run production models. Production models that incorporate broad regions of diverse data and compute 3D flow may be the only way to test ideas developed or conceived in investigation models, such as those regarding the flow in faults that we have just discussed. The investigation models are needed to keep production modeling a vital activity. Production modeling

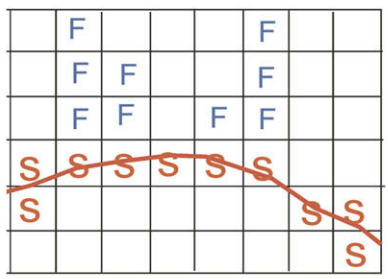

Fig. 7. Schematic of the CO_2 model. CO_2 is generated in the elements marked "S" as they cross (due to ongoing sedimentation) the 320 °C isotherm (the solid line). Overlying elements are "filled" with CO_2 if their Ca-, Fe- and Mg-alumino-silicates have all been titrated by interaction with previous packets of migrating CO_2 gas. These elements, marked "F", allow CO_2 to pass from the source to as-yet-unreacted elements or vent from the basin.

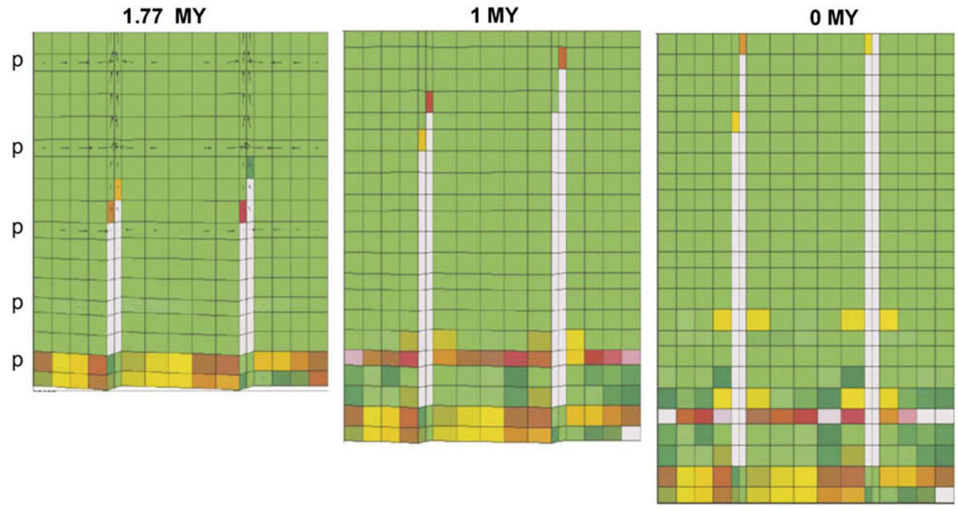

Fig. 8. Computed CO_2 generation, migration and titration in a simple basin with two permeable faults and 5 permeable strata marked "p". Light colors indicate CO_2 titration. By 0 Ma the fault to the right is venting CO_2 into the ocean, and the fault to the left is about to do so.

indirectly motivates and sustains investigation modeling. All the current production models have grown out of investigation models.

Looking to the future, some challenges are evident. When a field is new, as basin modeling was 20 years ago, it is relatively easy for an individual to develop a useful investigation model from scratch. Once a number of such models have been developed, however, it is increasingly difficult to justify building a new model from scratch, and the tendency is to use existing models as springboards, or run production models for scientific purposes. The entry-level effort required for an individual to build a new model that is fully comprehended becomes increasingly large, and the willingness of agencies to support such reinventions diminishes. But this, in time, risks that no one fully comprehends any of the current generation of investigation or production models. At the same time, as production models become more all encompassing and capable it becomes increasingly difficult to effectively discern and challenge aspects of their operation that may be questionable, and this is particularly true when there are no individuals passionately advocating scientifically-based aspects of models they fully comprehend. In this situation, modeling activity could eventually collapse to comparing predictions of currently existing codes with the idea that this can somehow identify risk and allow it to be managed. In proceeding along the current production and investigation modeling course we may risk extinguishing the scientific vigor of basin modeling.

How can this challenge be met? How can the scientific vitality of the basin modeling enterprise be sustained? How can the modeling energies of individual scientific investigators and the workers in the

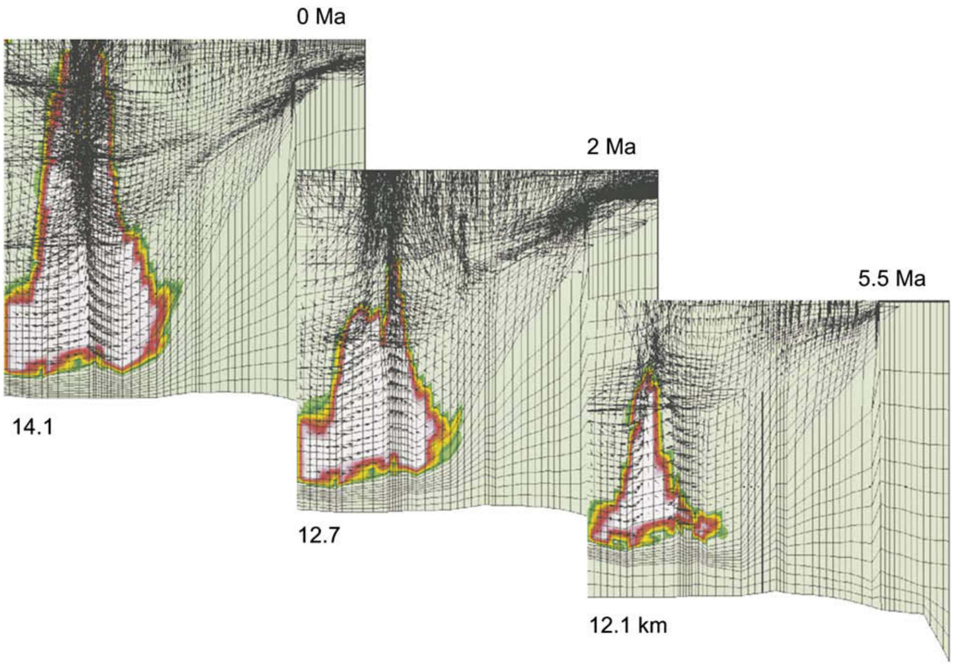

Fig. 9. Computed CO_2 generation, migration and titration in a section that runs from the center of the Yingghai basin in the South China Sea toward the northeast. The titration pattern (light colors) suggests that the risk of encountering high CO_2 mole fractions in gas reservoirs near the center of the basin is high, and this agrees with exploration drilling and production results.

Table 1
Two complimentary kinds of basin models.

Investigation	Production
Built by one person	Built by a group
Fully comprehended, little documented	Fully documented but lots hidden
Serially single purpose, publications	Broadly applicable, less publications
Flexible	Not very flexible
All variables accessible	Selected output
Generally user-unfriendly	Very friendly
Scientifically fertile	Ultimately scientifically sterile
Train geologists who may…	run production models
Pilot ideas which may…	be incorporated into production models
	only be tested in production models
Increasingly difficult to create and therefore vulnerable	Increasingly difficult to compete with and therefore isolated or monopolistic

companies that produce and maintain large production programs be utilized in ways that take the best advantage of the capabilities of everyone? One answer may be to encourage the encapsulation of modeling components into dynamic link libraries (DLLs or the equivalent) so that investigation and production models need not create all their own components from scratch, but can instead build on existing components or modules.

Dynamic link modules are simply encapsulated and accessible portions of code. They can be small code fragments or codes of broad modeling, analysis, and visualization capability. Their main requirement is a complete set of input parameters in a defined format and a complete and useful (to other modules) set of output products. In terms of our current discussion, one DLL module might accept a 3D description of litho-stratigraphy and fault locations and output the physical history of sedimentation, fault movement, and compaction. A fluid flow module could accept this output and compute the history of fluid flow. A chemical DLL could take the flow history and compute the chemical changes it would induce. A visualization DLL could read the output of any of the above modules and output images of the physical, flow, and chemical evolution of the basin. It could also compare the computed chemical change to field data if it had access to DLLs that could extract the field data.

Knowing the input and output protocols of each DLL, a researcher could write a DLL that would carry out new or different calculations or analysis and add to the collective capability, or explore an entirely new aspect of basin processes or data as part of a scientific investigation. Each DLL would need to be thoroughly tested and described, but the existence of a growing ensemble of such modules would take much of the duplicative work out of the basin modeling enterprise. More effort could be devoted to applying models to understand basin processes or to developing new modules. The increased effectiveness would encourage the involvement of young scientists and researchers in peripheral fields, and this would encourage advances that could aid basin resource exploration. If the modules were shared, industry and academic workers could collaborate free of management overhead. The modules would provide a natural bridge between all modeling groups.

To some degree what is described above is already happening. Freeware is increasingly providing useful component tools. The architecture of most basin modeling codes is of the nature described. Although there is not a clean or general separation of the modules that would allow the easy sharing of them with outside groups, today's codes are commonly nearly modularized already. So perhaps the question is how modularization and the sharing of modules, assuming it is desirable, could be facilitated.

The modular enterprise might be facilitated by workshops on how to create and use DLLs, the successful production of pilot models built by combining components, and the right kinds of incentives. It is time consuming and uncertain for a scientist that is not schooled in just the right aspects of computer science to learn, on their own, how to connect DLL modules. Workshops showing how this can be done would be valuable. A few examples of the successful combining of DLL components into useful basin models could be very stimulating. The idea seems good, but a few proof-of-concept examples would be much more persuasive. Researchers and software companies respond to incentives, and the enterprise could be facilitated if ways were found to give credits to those who develop or communicate the needed methods. The concept of basin modeling using a sea of well documented and understood yet inexpensive or freeware modules, and creating value mainly through their effective combination is new enough that it will take some time and/or encouragement to develop. But absent the development of this kind of environment, or something equivalent to it in function, the long-term (scientific and commercial) vitality of the basin modeling enterprise could be at risk.

4. Summary and conclusions

The movement of liquids and gases is fundamental to resource formation in basins and is recorded in chemical changes they induce. Incorporating inorganic and organic alteration into basin models could allow us to address fundamental questions of basin fluid flow, such as how fluids move in faults For example, the patterns of gas washing of oil and distribution of CO_2 mole fraction in reservoirs are accessible data sets, which, with the right kinds of models, could be inverted to reveal how faults have affected fluid movement. A great deal of science and technology will be required to construct the needed models. Complex geology must be incorporated, and accurate physical algorithms capturing thermal conductivity and compaction, chemical equations of state, and very large thermodynamic databases must all be available. To remain accessible to the entry of new scientists, and flexible enough to address new questions without unreasonable expense, the basin modeling enterprise should encapsulate as many modeling components as possible into DLL-type modules and place these modules in the public domain. Creating value by combining modules from this a sea of free modules would be a new style of business and science, but one that could keep basin science and technology vital for the foreseeable future.

Acknowledgements

I thank the organizers of the 2007 Hedberg Conference for stimulating the preparation of this paper, and two anonymous reviewers for suggestions that improved it. Funding by the DOE, the Gas Research Institute, Chevron, Texaco, and the Global Basins Research Network supported the work that forms the basis of its discussion.

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