geosciences

MDPI

Editorial

A Summary of "Future Advances in Basin Modeling: Suggestions from Current Observations, Analyses and Simulations"

Lawrence Cathles [1,*] and Willy Fjeldskaar [2,*]

1 Department of Earth and Atmospheric Sciences, Cornell University, Ithaca, NY 14853, USA
2 Tectonor AS, P.O. Box 8034, NO-4068 Stavanger, Norway
* Correspondence: lmc19@cornell.edu (L.C.); wf@tectonor.com (W.F.)

Received: 9 December 2020; Accepted: 18 December 2020; Published: 21 December 2020

1. Introduction

The objective of this volume differs from that of the usual review of current advances. While the state of the art remains the basis for departure, our main objective is to identify areas where advances in understanding and modeling could significantly impact exploration effectiveness. Our criterion is not what is the most exciting and important current science, but what could be the most important in the future. We encouraged our authors to avail themselves of the increased latitude for speculation that this future focus affords, and solicited the papers contained in this volume with this perspective.

A first step in any discussion of basin processes must be an observational appreciation of their scale and diversity. The scale of operation is huge, and the driving forces planetary. The first paper is an overview that reminds us of this. Subsequent papers address more specific basin phenomena:

- Two papers illustrate how changes in the stress tensor can be inferred and used.
- Two papers show how oil migration is impacted by glacial changes in strata tilt.
- Two papers calculate the delay in hydrocarbon maturation caused by salt diapirism.
- Three papers assess the impact of magmatic intrusion on the timing of hydrocarbon maturation and sediment alteration.
- Two papers address the progressive focusing of flow with distance traveled and how flow pathways can be detected seismically.
- One paper investigates the nature of compaction and alteration that is related to water flooding.
- Three papers describe and analyze basin hydrogen seeps and the possibility of a "new" nonhydrocarbon (H_2) basin energy resource.

2. Review of Volume Papers

2.1. Overview

In the first overview paper, Cathles [1] reminds us that basin formation is driven by global plate tectonics and that the basin fluids that accumulate resources can move over many hundreds of kilometers. Brine and petroleum fluid movements produce alteration patterns that can be vectors to resource accumulation. Flow can be steady or episodic. Different styles of flow produce different types of mineral and hydrocarbon resources. Permeability is not always an intrinsic property of a strata but is often dynamically controlled either by pressure or the presence of nonaqueous fluids. Shosa seals (the kind that can trap variably pressured gas for hundreds of millions of years) can massively fail and then reheal, repeatedly propelling large volumes of gas into subsurface aquifers. Seals can migrate through the stratigraphy, and porosity profiles record this migration and the causative pore pressure changes. Departures from the expected path of paleomagnetic pole migration may indicate the style of resource that should be sought in a basin. Basin processes are dynamic, diverse, and so large-scale that they are easy to overlook.

2.2. Stress

Who could guess that two weeks of outcrop mapping could reveal all the tectonic events that impacted the White Mountains over the last 410 Ma? Barton and Angelier [2] show how slip indicators on oriented outcrop faults can be inverted to identify the changes in the stress tensor that mark these events. The fresh, glacially exhumed New Hampshire outcrops are ideal for this purpose, but the dramatic success of the inversion suggests efforts to collect similar data (from drill holes, seismics, etc.) could quickly yield very valuable tectonic information.

The paper by Bouziat et al. [3] suggests one way this might be done. They determine the stress tensor by coupling a basin simulator with a finite element mechanical solver. Evaluating this method on a set of synthetic passive margin siliciclastic sediment accumulation histories, they predict the spatial–temporal pattern of stress tensor rotation and zones of weakness in the section from the growing sediment load and the changing basement tilt. For common basin parameters, the distal part of the sediment wedge is at all times compressive, the proximal part of the wedge is always extensional (but more so during lowstands), and areas of weakness develop under the continental slope late in the sedimentation history.

2.3. Reservoir Tilting

Many of the Earth's sedimentary basins are affected by glaciation. Repeated glaciations over the last millions of years have had great influence on the physical conditions in sedimentary basins and basin structure. Sedimentary basins near the former ice margin can be tilted enough to significantly alter the pathways of hydrocarbon migration. Løtveit et al. [4] present some of the major effects that ice sheets have on sedimentary basins by modeling data from the Norwegian part of the Barents Sea. Among the most important effects are movements of the solid Earth caused by glacial loading and unloading and related flexural stresses. Future basin models should include glacial loading/unloading when dealing with petroleum potential in former glaciated areas.

Cerroni et al. [5] describe a new model of the hydromechanical changes induced by a glacial cycle. They address the generation of the computational grid and the algorithm for the numerical solution. They present a multiscale approach that accounts for the global deformation of the lithosphere and couple it with the thermo-hydro-mechanical feedback of the ice load on a representative domain of smaller scale.

2.4. Salt Diapirs

Salt diapirs act as heat pipes and can depress temperatures in the nearby oil window by nearly 100 °C, delaying hydrocarbon maturation enough to affect exploration strategies. Two studies of the specific analysis of the impact of salt on basin temperature illustrate how the modeling of salt diapirs can be integrated into future exploration models. Cedeño et al. [6] used Slumberger software to analyze the impact of salt diapirism on the subsurface temperature and the timing of maturation in a confined salt-bearing basin in the Norwegian Barents Sea, showing that the densely packed diapirs depress temperatures by 50–70 °C and delay maturation. With examples from the Nordkapp Basin, they show that the temperatures along the diapir flanks are 70 °C cooler and are exceptionally low (~150 °C) at depths of ~9 km beneath the salt.

Grunnaleite and Mosbron [7] show that salt structures on the Eastern flank of the Central Graben of the Norwegian North Sea depress temperatures by 85 °C and vitrinite R_o by up to 1.0%. They use the BMT (Basin Modeling Toolbox) software to accurately track the changing shape of the diapirs (especially the retraction of the root), and present what may be the most realistic salt model of a specific site yet published. They show the timing and geometrical evolution of salt structures depends critically on correctly defining the geometry of salt volumes and having a good geohistory model.

2.5. Magmatic Sills

Magmatic sills can increase the temperature of organic-rich strata and cause them to mature earlier than otherwise expected. Brown and Kim [8] set the stage by reviewing crustal reflection profiling seismic data to show how common sills are in the crystalline crust that underlies all basins. These sills can transfer heat from the mantle, change crustal rheology, and potentially affect overlying basin evolution in a fashion that impacts hydrocarbon and mineral resource potential.

Sydnes et al. [9] report the results of a sensitivity study of the impact of sills on temperature and maturation when attendant faulting is taken into account. They show that omitting structural changes related to magmatic intrusion may lead to over- or underestimation of the thermal effects of magmatic intrusions and the timing of maturation.

Sydnes et al. [10] evaluate the impact of sill emplacement on diagenetic processes and stress accumulations. Based on data from the Vøring Basin (Norwegian Sea), the modeling shows that basins with magmatic intrusions have thermal histories that enhance diagenetic processes during and after sill emplacement. Areas located between clusters of sills are particularly prone to diagenetic changes. The chemical alteration changes the stress pattern.

2.6. Fluid Flow

Fluids transport and concentrate all resources. Understanding and identifying the pathways of flow is perhaps the most important challenge for the explorationist. Two fundamental questions arise: First: how are the flow pathways likely to change with the distance of flow? Second: particularly if the pathways are increasingly concentrated, where are they located in a specific subsurface volume? Malin et al. [11] address the first question by showing that two factors control whether flow will concentrate with distance traveled: the spread (standard deviation) of log permeability about its mean, and whether permeability is distributed in a scale-invariant fashion. If the spread is substantial and the distribution scale invariant, flow will become increasingly concentrated with distance traveled. The spread of permeability is notoriously large, and fractures are scale-invariant in their distribution. This is a matter of observation. The reason is probably that the Earth's crust is in a state of near failure and scale-invariant systems are commonly observed near the critical point of failure. Knowing that flow is likely concentrated in any particular volume is a good perspective, but of little use if the actual flow channels in the volume cannot be located.

Sicking and Malin [12] describe how subsurface flow channels can be located from the seismic energy emitted by Krauklis waves trapped on water-filled fractures. The contrasting seismic wave velocity between water in the fractures and the surrounding rock traps seismic energy, and seismic waves bounce back and forth from the ends of the fracture. Episodes of harmonic humming, often minutes or more in duration, can be extracted from what is usually considered seismic noise using specialized processing techniques. Permeable channels are presumed to be where fluid-filled fractures are most abundant. A substantial number of field studies support this hypothesis. Necessary analysis can be carried out by processing existing 3D seismic data.

2.7. Chemical Alteration

Compaction is important in basin models; decompaction is an indispensable step in their construction. Compaction is of practical importance in Norwegian North Sea petroleum production. The Ekofisk platform has subsided 9 m over 40 years. Half of this subsidence is due to production-related decreases in pore pressure, which can be arrested by maintaining reservoir pressure; but half is due to the injection of water for secondary hydrocarbon recovery, which results in a slow plastic creep that declines with time and is independent of the elastic compaction that immediately attends changes in pore pressure (effective stress). Minde and Hiorth [13] analyze this second kind of creep compaction, first in terms of sliding block observations, and then in terms of water chemistry and chemical alteration. Sliding blocks slip at a declining rate after the initiation of slipping because the contact surface area between them increases with time. Creep experiments can be interpreted similarly for the slip between grains. The activity of water affects this creep.

When SO_4 is present in the pore fluid, creep is faster than expected from the sliding block model. This is because sulfate ions make the surface charge of calcite much more negative and produce a disjoining (osmotic) pressure, which pushes the grains apart and weakens the chalk. Flooding with $MgCl_2$ causes still more rapid compaction: three times more rapid than flooding with sulfate. This is because during the core flooding calcite is replaced volumetrically with magnesite, which is 10% more dense. Chalk creep compaction is thus due to at least three factors: changes in grain contact area, changes in the surface charge of calcite, and chemical replacement reactions. Translating from the laboratory to the reservoir requires taking into account the movement of the thermal front associated with the injection of cold seawater and chemical reactions tied to this thermal front, as well as the changes in water salinity (displacement of connate brine with injected seawater) that move more rapidly through the reservoir. Minde and Hiorth [13] show how careful interpretations of reservoir production phenomena identify concepts that might be transferred to more sophisticated future basin models.

2.8. H_2 Basin Resources

The last three papers discuss a completely new and surprising kind of nonhydrocarbon basin energy resource. Hydrogen gas has been observed venting from circular depressions (fairy circles) in many basins. As described by Cathles and Prinzhofer [14], H_2 concentrations at 1 m depth in the Sao Francisco Basin in Brazil occur mainly at the margins of a circular depression ~550 m in diameter, and are nonzero for about 6 h a day with peak concentrations occurring at ~1:00 pm. The periodic venting could be caused by atmospheric pressure tides, which have a very regular diurnal cycle at this location. The maximum rate of atmospheric pressure decrease occurs at 1:00 pm. The changing atmospheric pressure pushes air into and pulls it out of the subsurface in an accordion-like fashion. The volume of the gas pulled in and out of the shallow subsurface vents must be 1000 times less than the volume of gas in the subsurface reservoir that is compressed and decompressed. H_2 losses to the atmosphere can be supplied by a H_2 flux of ~0.1 $m^3\ m^{-2}\ d^{-1}$.

Donzé et al. [15] address the critical question of whether the H_2 venting observed in many basins could constitute a significant energy resource by placing the venting rate analyzed by Cathles and Prinzhofer in contest with the local geology and global venting rate estimates. The H_2 generation rate expected from the 10^8 km^2 of Precambrian lithosphere, scaled to the 300,000 km^2 area of the Sao Francisco basin, suggests the entire basin could generate 90 to 266 tons H_2/y by radiolysis and/or 113 to 1018 tons H_2/y by serpentinization. Both generation mechanisms are possible in and under the Sao Francisco Basin: faults cut deeply into the crust, and storage reservoirs are present. However, the H_2 venting rate estimated by Cathles and Prinzhofer of 200 to 5400 tons H_2 per year from a single vent is as high as that expected from the entire Sao Francisco Basin, which suggests either the global estimates are too low or the venting at the study site is presently unusually strong.

Finally, Simon et al. [16] discount the possibility that solid Earth tides could be the cause of the variable venting in the Sao Francisco Basin by showing that solid Earth tides at the site have two co-equal peaks per day, but the H_2 venting has only one. We are just beginning to understand the H_2 system. We are at a stage similar to when we knew of a few hydrocarbon seepages, but had no concept of the magnitude or importance of the petroleum system.

3. Discussion

Perhaps what stands out most from the papers in this volume is the magnitude of the challenge of properly incorporating the diverse basin processes into models that can be usefully deployed to analyze basins in a resource context. The application papers in this volume indicate the potential of this. Capturing the stratigraphy, faulting, and salt diapirism realistically impacts the timing of hydrocarbon maturation and suggests the pattern of metamorphic alteration. Calculating stress changes from sediment loading predicts the locations of rock failure (fracturing). Strata tilting, sediment compaction, and fluid flow driven by glaciers can be analyzed with important resource implications. However, the effects of magmatic sill intrusion (even in the basement) can change everything, and assuming pressure depends on regular compaction is probably inappropriate. The movement of Shosa-type capillary seals can shift the pattern of overpressuring and fluid flow, and nonlinear stress feedbacks can be expected from alteration, faulting, and slumping. Identifying and properly incorporating all the process interactions will be very challenging.

The flip side of this incorporation challenge is the insights that can be obtained from diverse observations. Compaction is a process that changes physically with grain comminution and with the chemical activity of water, water chemistry, and rock alteration. Insights from investigations of the subsidence of oil platforms can be transferred to future basin models. Chemical alteration tied to water flooding can be transferred to mineral exploration basin models.

Basins reflect physical fundamentals, and the fundamentals pose powerful constraints. The scale invariance of strata and fractures, a consequence of the state of incipient failure of the atmosphere and lithosphere, indicates that the progressive channeling of fluid flow with distance traveled must be expected. It is thus of the greatest significance that subsurface permeability might be mapped by the intensity of seismic energy trapped on fluid-filled fractures. The ability to define the permeability structure at a specific site could change resource exploration in the most dramatic and exciting fashions.

Basins are giant thermo-chemical-structural reactors that produce mineral and diverse hydrocarbon resources. Hydrogen, seeping from Proterozoic basins worldwide, is a basin energy resource that combusts only to water vapor and generates no CO_2. The size and significance of this resource is yet to be determined, but the periodicity of venting reveals much about near-surface permeability and reservoirs of H_2.

New ground is cut by nearly all the papers in the volume. Shosa seals have many important implications. The pulses of flow they allow can reset the paleomagnetic pole on a subcontinental scale. Fault slip and other stress change-related observations are most powerful if interpreted as temporal changes in the stress tensor. Glaciation can tilt strata sufficiently to change the directions of petroleum migration. Sill intrusions are common in basins and the underlying lithosphere, and can change temperature and stress. There is a fundamental tendency for flow to become increasingly channelized with distance traveled. Seismic waves trapped in fluid-filled fractures indicate flow channels. Grain comminution, changes in water activity, aqueous chemistry-related changes in surface change, and replacement reactions all contribute to reservoir creep compaction. The H_2 system is a new and exciting kind of basin energy resource whose significance is yet to be defined.

The papers in this volume by no means cover all the topics that could be of interest and significance in basin modeling. We would, for example, have liked to include papers on gas adsorption and desorption. Gas seepages in glaciated areas may reflect the release of absorbed gas following the very recent glacial unloading (Jay Leonard, pc 2018). Hydrocarbon alteration during migration is touched upon in the overview, but gas washing is only one part of this important phenomenon, and it would have been nice to have a good overview paper summarizing what is known and what is not about organic chemical changes related to phase fractionation (the separation of supercritical gas–oil into distinct gas and oil phases), gas condensation, mixing, and bacterial and thermal degradation. Secondary hydrocarbon migration is also not treated at all in this volume. Crustal flexure is important in basin margins, and there is much yet to be learned from observed deformation patterns.

There is surely also much that is important that we do not currently perceive. As a community, we have stumbled over some things that could have been obvious much earlier (such as the potential significance of glacial tilting). We have addressed H_2 venting enough to recognize that we know almost nothing about the importance of this noncarbon energy system. We know a bit about the CO_2 generation–migration–trapping system in basins, but there are probably other chemical systems that are of significance. It would be wonderful to know more about the general chemical chromatography of basins.

Basins host mineral and nonhydrocarbon energy resources that will be important in the future. Knowledge of basins, in part an important heritage of the hydrocarbon era, provides a strong foundation, yet there is a lot that remains to be learned about the thermo-chemical-structural reactors we call sedimentary basins. The future is very bright for the next generation of researchers that will seek to address basin processes and resources. We hope that this volume will stimulate enthusiasm and encourage the research into basin resources that is necessary to meet the mineral and energy needs of the future.

Author Contributions: The authors contributed equally to the preparation of this summary. Both authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: All data in this review is contained in the volume papers reviewed.

Acknowledgments: The authors thank all the scientists who contributed their high-quality papers to this volume, and the regular editors of *Geosciences* who made the submission and review process for the guest editors and authors very easy.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Cathles, L. On the Processes that Produce Hydrocarbon and Mineral Resources in Sedimentary Basins. *Geosciences* **2019**, *9*, 520. [CrossRef]
2. Barton, C.C.; Angelier, J. Direct Inversion Method of Fault Slip Analysis to Determine the Orientation of Principal Stresses and Relative Chronology for Tectonic Events in Southwestern White Mountain Region of New Hampshire, USA. *Geosciences* **2020**, *10*, 464. [CrossRef]
3. Bouziat, A.; Guy, N.; Frey, J.; Colombo, D.; Colin, P.; Cacas-Stentz, M.-C.; Cornu, T. An Assessment of Stress States in Passive Margin Sediments: Iterative Hydro-Mechanical Simulations on Basin Models and Implications for Rock Failure Predictions. *Geosciences* **2019**, *9*, 469. [CrossRef]
4. Løtveit, I.F.; Fjeldskaar, W.; Sydnes, M. Tilting and Flexural Stresses in Basins Due to Glaciations—An Example from the Barents Sea. *Geosciences* **2019**, *9*, 474. [CrossRef]
5. Cerroni, D.; Penati, M.; Porta, G.; Miglio, E.; Zunino, P.; Ruffo, P. Multiscale Modeling of Glacial Loading by a 3D Thermo-Hydro-Mechanical Approach Including Erosion and Isostasy. *Geosciences* **2019**, *9*, 465. [CrossRef]
6. Cedeño, A.; Rojo, L.A.; Cardozo, N.; Centeno, L.; Escalona, A. The Impact of Salt Tectonics on the Thermal Evolution and the Petroleum System of Confined Rift Basins: Insights from Basin Modeling of the Nordkapp Basin, Norwegian Barents Sea. *Geosciences* **2019**, *9*, 316. [CrossRef]
7. Grunnaleite, I.; Mosbron, A. On the Significance of Salt Modelling—Example from Modelling of Salt Tectonics, Temperature and Maturity Around Salt Structures in Southern North Sea. *Geosciences* **2019**, *9*, 363. [CrossRef]
8. Brown, L.D.; Kim, D. Extensive Sills in the Continental Basement from Deep Seismic Reflection Profiling. *Geosciences* **2020**, *10*, 449. [CrossRef]
9. Sydnes, M.; Fjeldskaar, W.; Grunnaleite, I.; Løtveit, I.F.; Mjelde, R. Transient Thermal Effects in Sedimentary Basins with Normal Faults and Magmatic Sill Intrusions—A Sensitivity Study. *Geosciences* **2019**, *9*, 160. [CrossRef]
10. Sydnes, M.; Fjeldskaar, W.; Grunnaleite, I.; Løtveit, I.F.; Mjelde, R. The Influence of Magmatic Intrusions on Diagenetic Processes and Stress Accumulation. *Geosciences* **2019**, *9*, 477. [CrossRef]
11. Malin, P.E.; Leary, P.C.; Cathles, L.M.; Barton, C.C. Observational and critical state physics descriptions of long-range flow structures. *Geosciences* **2020**, *10*, 50. [CrossRef]
12. Sicking, C.; Malin, P. Fracture Seismic: Mapping Subsurface Connectivity. *Geosciences* **2019**, *9*, 508. [CrossRef]
13. Minde, M.W.; Hiorth, A. Compaction and Fluid—Rock Interaction in Chalk Insight from Modelling and Data at Pore-, Core-, and Field-Scale. *Geosciences* **2019**, *10*, 6. [CrossRef]

14. Cathles, L.; Prinzhofer, A. What Pulsating H_2 Emissions Suggest about the H_2 Resource in the Sao Francisco Basin of Brazil. *Geosciences* **2020**, *10*, 149. [CrossRef]
15. Donzé, F.-V.; Truche, L.; Shekari Namin, P.; Lefeuvre, N.; Bazarkina, E.F. Migration of Natural Hydrogen from Deep-Seated Sources in the São Francisco Basin, Brazil. *Geosciences* **2020**, *10*, 346. [CrossRef]
16. Simon, J.; Fulton, P.; Prinzhofer, A.; Cathles, L. Earth Tides and H_2 Venting in the Sao Francisco Basin, Brazil. *Geosciences* **2020**, *10*, 414. [CrossRef]