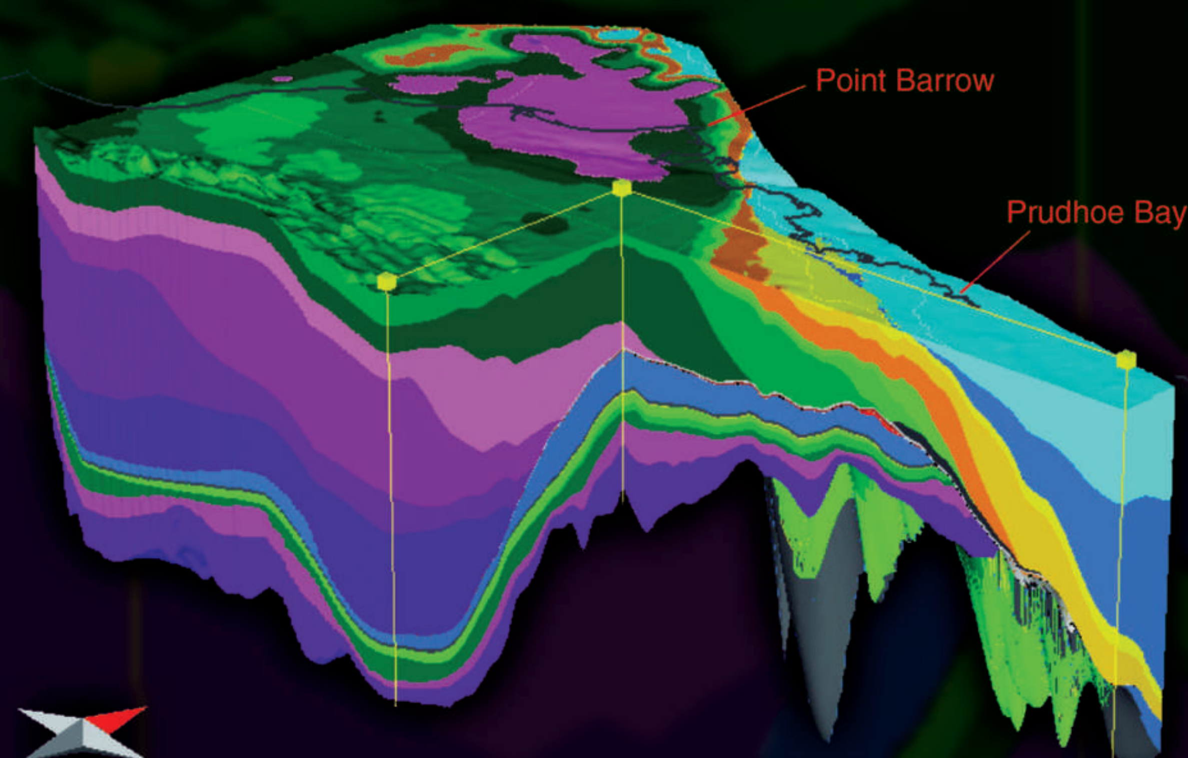
AAPG Hedberg Series 4

Basin Modeling:

New Horizons in Research and Applications



Edited by Kenneth E. Peters, David J. Curry, and Marek Kacewicz

Basin Modeling: New Horizons in Research and Applications

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COVER: Present-day geometry of the Alaskan North Slope petroleum system modeling study (Schenk et al., pg. 317) with north-south cut-planes showing the slope from the Barrow Arch toward the foothills of the Brooks Range and west-east cut-planes along the Barrow Arch pointing to the Prudhoe Bay structure.

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About the Editors

Kenneth E. Peters is science advisor for Schlumberger Information Solutions (SIS) where he uses geochemistry and numerical modeling to study petroleum systems. He has more than 32 years of experience working for Chevron, Mobil, ExxonMobil, USGS, and Schlumberger and has taught petroleum geochemistry and basin modeling at Chevron; Mobil; ExxonMobil; Oil & Gas Consultants International; University of California Berkeley; and Stanford University. Ken is principal author of *The Biomarker Guide* (2005, Cambridge U. Press) and consulting professor in the Geological and Environmental Sciences Department at Stanford University where he leads the Basin and Petroleum System Modeling Industrial Affiliates Program. He was chair of the AAPG Research Committee (2007–2010), AAPG Distinguished Lecturer for 2009 and 2010, and editor for the 2009 AAPG compact disk *Getting Started in Basin and Petroleum System Modeling*. He is an associate editor for *AAPG Bulletin* and *Organic Geochemistry*. In 2009, he received the Schlumberger Henri Doll Prize for Innovation and the Alfred E. Treibs Award presented on behalf of the Organic Geochemistry Division of the Geochemical Society to scientists who have had a major impact on the field of organic geochemistry through long-standing contributions. Ken has B.S. and M.S. degrees in geology from University of California, Santa Barbara and a Ph.D. in geochemistry from University of California, Los Angeles.

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Marek Kacewicz is research consultant and basin modeler at Chevron Energy Technology Company in Houston, Texas. His primary responsibilities include technology applications and research integrating petroleum systems modeling, seismic inversion, velocity modeling, pressure prediction, geomechanics, and structural modeling. Prior to Chevron, Marek worked as a research geologist at ARCO Exploration and Production Research Center in Plano (Texas, USA); as a basin modeler at Unocal Exploration & Exploitation Technology in Sugar Land (Texas, USA); Alexander von Humboldt Fellow at the Freie Universitaet Berlin (Berlin, Germany); and research assistant at the University of Warsaw (Warsaw, Poland). Marek has over 20 years of experience in petroleum systems modeling, exploration, and research. His experience includes both conventional and unconventional resources and covers a wide range of sedimentary basins worldwide. Some of Marek's professional honors include receiving the 1986 International Association for Mathematical Geology Vistelius Research Award, being selected for the Alexander von Humboldt Fellowship (Germany); and receiving the 2005 AAPG Gabriel Dengo Memorial award. He has an M.S. degree in numerical mathematics/computer science and a Ph.D. in earth sciences, both from the University of Warsaw (Poland).

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Introduction

An Overview of Basin and Petroleum System Modeling: Definitions and Concepts

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ABSTRACT

This special volume contains a selection of articles presented at the AAPG Hedberg Research Conference on Basin and Petroleum System Modeling (BPSM) held in Napa, California, on May 3–8, 2009. These articles provide an overview of the current state of the science. The main purpose of the conference was to facilitate the exchange of ideas and enhance cooperation among the leading experts from industry, academia, and government to improve modeling concepts, tools, and workflows required to optimize exploration and production. Kacewicz et al. (2010) summarize the conference proceedings and findings. This conference was a direct result of the previous heavily oversubscribed and highly successful Hedberg Conference on Basin Modeling held in the Netherlands (May 6–9, 2006), at which the Dutch organizers suggested the need for another meeting on the same topic within 2 to 3 yr, preferably in North America.

The substantial target audience for this volume consists of (1) geochemists and BPSM modelers in industry, government, and academia; (2) geoscientists with interest in region-specific BPSM studies; and (3) specialists in different geoscience disciplines that are significant to the development of BPSM input parameters and simulation algorithms. Basin and petroleum system modeling is one of the most rapidly growing disciplines within the geosciences because of the high demand by industry for continuous improvement in predictions of petroleum generation, migration, accumulation, and alteration. Virtually all major oil companies now have substantial geochemistry and BPSM groups.

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INTRODUCTION

Basin and petroleum system modeling (BPSM) is a rapidly growing research and application tool that spans many disciplines within the geosciences (Hantschel and Kauerauf, 2009). The principal aim of BPSM is to reduce the risk associated with exploration, production, and development of petroleum. The purpose of this chapter is to introduce the articles from those sessions included in this volume, describe some of the basic concepts of BPSM, define key terms, and provide an overview of some future directions for this multidisciplinary research.

Although many workers use the term ''basin modeling'' to include petroleum system modeling, basin modeling and petroleum system modeling are different. In basin modeling, mathematical equations are used to reconstruct the deposition, compaction, and erosion of rock layers through time and space and the concomitant evolution of the thermal history of the basin. Although basin modeling deals with rocks, petroleum system modeling deals with hydrocarbon fluids. Hydrocarbons are composed mainly of hydrogen and carbon, especially thermogenic oil and gas, but also including biogenic methane. The term ''petroleum system'' is commonly misused, although it is rigorously defined. A petroleum system consists of all the elements and processes responsible for accumulations and all of the genetically related petroleum that originates from one pod of active source rock (Magoon and Dow, 1994). Of course, the petroleum industry is mainly interested in the hydrocarbon fluids, but to model petroleum systems, one must first model the rocks and their geologic histories.

Basin and petroleum system modeling uses forward deterministic computations to simulate the thermal histories of the rocks and the related generation, migration, and accumulation of petroleum, that is, processes are modeled from past to present using inferred starting conditions (Figure 1). These computations require a conceptual model of basin history that has been subdivided into an uninterrupted sequence of events in space and time, including the deposition and erosion of rock units. Model simulations are performed on discretized numerical representations of the available geologic and geochemical data, that is, spatial data are subdivided into grid cells having constant property distributions within each cell. For example, a grid cell might measure 1 km (0.6 mi) on each side and 400 m (1312 ft) in thickness. Numerical values are required for all input parameters in Figure 1. Input data include gridded surfaces of buried rock units from seismic and well-log interpretations, ages of units, present and past rock unit thicknesses, structural restoration through time, lithology and physical properties of units, porosity, permeability, and various boundary conditions, such as present and past water depths, basal heat flow, and sediment-water interface temperatures. The type and amount of organic matter in the source rocks and the kinetics for the conversion of source rock organic matter to petroleum are also required. Model output, such as predicted temperature, pressure, or porosity, can be compared with independent calibration parameters, thus allowing the conceptual model to be adjusted to improve the match between the calibration data and simulation output.

During the last decade, the value and advantages of BPSM have become widely recognized throughout the geoscience community because BPSM can:

1. Organize and archive input data, for example, subsurface structure from seismic surveys, lithology, and present-day temperature from well logs, paleowater depth, and formation age from micropaleontology, heat flow interpreted from tectonic history, and organic richness and thermal maturity from geochemical measurements
2. Help to quantify the essential risk elements (source, reservoir, seal, and overburden) and processes of the petroleum system (trap formation and generation-migration-accumulation; Magoon and Dow, 1994) and focus further work
3. Quantify key petroleum system elements and processes that control petroleum generation, migration, and accumulation within basins, which helps to focus work on the parameters that most affect simulation results
4. Convert raw seismic, geochemical, and geologic data to interpretations that can be tested to assess the range of possible model outcomes
5. Provide a consistent approach to rank or risk prospects and to allocate appropriate levels of professional staff or resources

DISCUSSION

This book consists of six sections similar to those in the conference. The articles in each section are briefly described.

Geochemistry: Challenges in the Future

Clement N. Uguna et al. conducted high-temperature, high-pressure experiments in supercritical water (as high as 420°C) to achieve high thermal maturities (vitrinite reflectance [R_o], >2% R_o) for samples of Upper Jurassic Kimmeridge Clay source rock. Pressures between 390 and 500 bar, the highest used, retard both hydrocarbon generation and maturation after the well-documented promotional effects of water on maturation reach a maximum at 200 to 300 bar. The results provide further evidence that the first-order

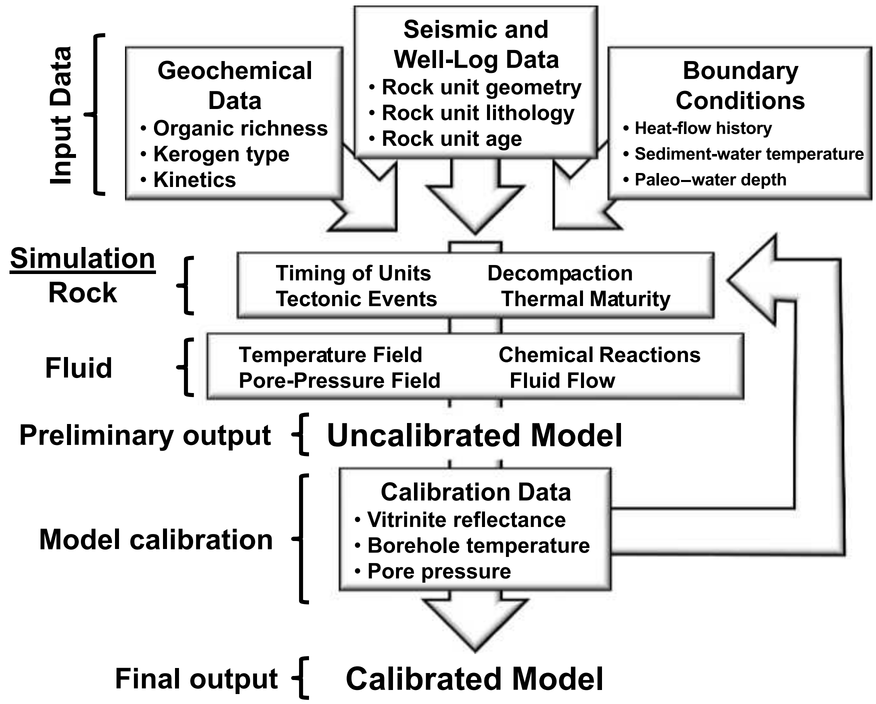

FIGURE 1. Process workflow for basin and petroleum system modeling (from Peters, 2009).

kinetic models used in petroleum system modeling need to incorporate the effects of pressure.

Frank Haeseler et al. present the results of a compositional model called BioClass 0D that predicts total hydrocarbon losses and the residual composition of biodegraded oil. This model was applied to three nonbiodegraded oils representative of the source rocks that contain the three main types of organic matter: types I, II, and III.

Frederic Schneider et al. show that more care should be exercised in the determination of kinetic parameters for source rocks to account for phenomena that occur in the diagenetic zone (<0.6% R_o). Petroleum system models that use kinetic parameters determined on samples at the end of the diagenetic zone (~0.6% R_o) underestimate the amounts of hydrocarbons produced.

Seismic/Pressure/Gravity Magnetics Revisited

Heinz-Juergen Brink et al. used the common reflection surface (CRS) stack technique for reprocessing seismic data to better image the Moho and support an alternate view of the geodynamic origin of the North German Basin. The data allow a revised interpretation of the structural setting and evolution of different salt features in the basin and yield new insights into petroleum systems in the basin.

Frederic Monnier et al. used local grid refinement (LGR) to better define key areas within a larger regional model from northern Kuwait, where they compared it with other refinement methods. The study illustrates the linkage of LGR and compositional three-dimensional (3-D) Darcy flow modeling to predict the distribution of hydrocarbon composition and properties in local reservoir rock areas, where accumulations were predicted. The LGR approach bridges the gap between conventional basin modeling and reservoir modeling and was used to predict API gravities, gas/oil ratios, and the oil-water contact in new prospects.

Structural and Tectonic Processes

Richard Gibson outlines a simple method to realistically describe variations in subsurface salt geometry through time and shows how to implement these variations into basin models without requiring full 3-D structural restoration as an input. This approach was used to produce a basin-scale numerical simulation model of the northern Gulf of Mexico that restores back through time with minimal geometric artifacts, despite complex structural geometries.

Carolyn Lampe et al. studied the Brooks Range Foothills in Alaska using a new approach to integrate three classic disciplines of modeling: structural balancing, fault property analysis, and BPSM. The combination of these disciplines improves understanding, assessment, and prediction of the extent, timing, and generative potential of petroleum systems in tectonically complex areas.

Susanne Nelskamp et al. combined structural modeling with petroleum system modeling in a two-dimensional section of the Dutch onshore region. The model results demonstrate the effects of tectonic inversion, erosion, and subsidence on the geohistory of the thermal field and petroleum generation.

New-Generation Methods/ Unconventional Approaches

Jan Derks et al. describe a local grid refinement method that combines regional-scale petroleum system models and local reservoir- or prospect-scale models. The method was applied to an oil field in Kuwait, where heavy oil zones occur at the original oil-water contact and also in stratigraphic and structural positions above it. The study demonstrates that the heavy oil distribution in those layers can be explained by the petroleum charge history.

Hanneke Verweij et al. modeled the geohistory of the Terschelling Basin and the southern part of the Dutch Central Graben by incorporating a tectonic heat flow boundary condition and detailed knowledge of Tertiary climate changes. The 3-D simulation shows a marked difference in generated hydrocarbon volumes and a shift in the timing of Tertiary petroleum generation compared with simulations using a default surface temperature boundary condition based on paleolatitude reconstruction. The results improved understanding of the thermal maturity and timing of hydrocarbon generation from the Jurassic and Carboniferous source rocks.

Sylvie Wolf et al. developed a new time-stepping method to model oil generation in sedimentary basins based on separating pressure from oil saturation. The method is capable of yielding accurate solutions compared with those computed by the fully implicit scheme, but with an effective reduction of computation time by as much as a factor of five.

Uncertainty in Basin Modeling

Paul Hicks et al. present a basin modeling workflow to identify key input parameters and to quantify uncertainties in these input parameters to evaluate the model results in light of a business question. They demonstrate this workflow using a hypothetical case in which uncertainties in key input parameters that control hydrocarbon generation, volumes, and timing are identified, quantified, and propagated through a basin model.

Sylvie Pegaz-Fiornet et al. focus on the Darcy and invasion percolation approaches to quantify secondary and tertiary petroleum migration and compare the advantages and limitations of each method. The Darcy method accounts for buoyancy, capillary pressure, pressure gradients, and transient physics. The calculation can be time consuming, but it provides a good description of caprock leakage. Invasion percolation is less comprehensive than the Darcy method, but the calculation is faster, and it is especially useful to simulate secondary migration.

Noelle Schoellkopf describes the role of the basin modeler in new ventures exploration risk assessment. Although we can rank model input parameters, such as fetch area, depth, source thickness, total organic carbon (TOC), hydrogen index (HI), temperature gradient or heat flow, and the impact on fluid phase and volumes, we should be aware of pitfalls. Underlying geologic assumptions may account for the greatest uncertainty in new basin areas, where data are sparse and models are poorly calibrated. Modeling tools must be flexible enough to allow multiple working hypotheses within the project timeframe. These hypotheses are best evaluated by an integrated project team that includes a basin modeler.

Andre Vayssaire examines the premise that kilometer-scale vertical migration through fine-grained sediments is the principal mode of transport for hydrocarbons from source rock to reservoir in the Malvinas Basin of Argentina. He compares simulation results based on Darcy flow with those of invasion percolation methods. Based on physics, Darcy flow is more appropriate to simulate kilometer-scale hydrocarbon migration across fine-grained sediments. However, the relative permeability curves need to be upscaled to mimic a migration process that likely occurs along thin stringers. Under these conditions, viscous forces can be ignored, and the invasion percolation method seems to be more appropriate.

Case Studies and Workflows

Friedemann Baur et al. show that gas/oil ratios and API gravities of petroleum accumulations in the Jeanne d'Arc Basin, offshore eastern Canada, can be accurately reproduced by 3-D numerical models that use multicompositional phase-reproducing reaction kinetics measured on samples from the Egret Formation source rock. The chapter reconstructs the detailed filling history of the Terra Nova oil field and deduces the locations of the kitchen areas based on mass-balance calculations and migration pathway analysis.

John Guthrie et al. used one-dimensional and multisurface thermal modeling to help resolve the effects of hydrocarbon charge timing, charge rate, timing of trap formation, and reservoir temperature history on the quality of oil in reservoirs of the Roncador and Frade fields, offshore Campos Basin, Brazil. An interactive biodegradation tool in the modeling software was used to predict API gravity, and the results are constrained by the geology and the geochemical composition of the present-day fluids in the reservoirs.

Oliver Schenk et al. present a detailed 3-D BPSM study of the North Slope of Alaska (275,000 km^2 [106,178 mi^2]) designed to reduce exploration risk and assess remaining petroleum potential. The model is based on more than 48,000 km (29,826 mi) of seismic data and formation top, geochemical, and calibration data from more than 400 wells. The study includes reconstruction of complex basin paleogeometry, including diachronous deposition of overburden rock and several localized erosion events.

CONCLUSIONS

It is appropriate to end this introduction with a brief discussion of several key topics where further research might significantly improve the use of BPSM. A more comprehensive list of targeted research topics is available in the summary of the conference proceedings (Kacewicz et al., 2010).

Basin and petroleum system modeling can be used to accurately predict the extent of the pod of active source rock and the thermal maturity and timing of petroleum generation from that source rock. It is currently less useful to predict volumes of trapped petroleum, their detailed compositions, or the effects of postgeneration processes, such as biodegradation. However, improved prediction of these parameters could have a major impact on domestic and world economies. Basin and petroleum system modeling will continue to expand because of the potential for high-impact solutions to these problems with respect to exploration, development, and assessment.

Modeled predictions of the volumes and compositions of trapped petroleum are limited by current understanding of migration efficiency out of the source rock and from the source rock to the trap. This gap in knowledge will become even more evident with increased exploration for unconventional resources, such as shale gas and shale oil. Further research is needed to better understand the heterogeneity, geochemistry, and mechanical properties of source rocks and how these influence the expulsion and retention of hydrocarbons. This research will require the integration of many disciplines, including seismic lithofacies analysis, sedimentary petrology, geochemistry, petrophysics, rock mechanics, and BPSM. Readers will note that one deficiency in this volume is a lack of articles on rock properties and lithofacies distributions. More studies are needed to improve the link between seismic lithofacies analysis and model input. Lithofacies distributions are rarely known, so better integration of BPSM and basin filling software is needed. Although the properties of clastic rocks have been studied for some time, carbonate source rocks and migration through carbonate carrier rocks deserve much more attention.

Rates of petroleum generation are controlled by kinetic parameters for the organic matter in different source rocks, which in many studies are poorly known because of the lack of adequate rock samples for kinetic measurements. Further study is needed to investigate the potential of asphaltenes isolated from oil samples to infer source rock kinetics. In addition, most models are calibrated using R_o and corrected bottomhole temperatures. In the future, more compositional kinetic models will be calibrated using measured reservoir pressures and the compositions of reservoir fluids. This will require further development of algorithms to address secondary processes that affect petroleum composition, including biodegradation, thermochemical sulfate reduction, and secondary cracking in the source and reservoir rocks.

Simulation of fluid migration through faults requires more research. Most simulators treat fault behavior as input. For example, faults can be designated by the user as open or closed during various time intervals. Deterministic models are needed that predict evolving fault behavior with respect to migrating fluids. This goal can only be achieved by parallel development of viable 3-D rock movement simulators. Current simulators are designed to model vertical rock movement, including burial, uplift, and insertion or removal of salt layers. However, an urgent need for 3-D simulators that can routinely reconstruct nonvertical rock movement, such as thrust faulting, exists.

Despite recent advances in computing speed, personal computers remain inadequate for complex petroleum system models, especially those designed to evaluate risk based on several parameters having large uncertainties. Computations involving large models will continue to be impractical without the speed offered by parallel processing. Nevertheless, continued advances in computing power will allow more models to be conveniently run using personal computers. Expanded options for uncertainty analysis are needed in most simulators, such as uncertainty-related subsurface geometry or the ages of sedimentary units.

GLOSSARY

The purpose of the following glossary is to assist readers of this volume who may have various levels of expertise in basin and petroleum system modeling. The glossary draws upon definitions in Peters and Cassa (1994), Magoon (2004), and Peters et al. (2005). As much as possible, the glossary includes terms directly relevant to basin and petroleum system modeling and excludes terms that are familiar to most geologists.

Activation energy

The energy required for chemical transformations, commonly expressed in kilocalories per mole or kilojoules per mole. Activation energy distributions are used in maturation modeling to calculate the degree of transformation of kerogen in the source rock to oil and gas (Baur et al., Section VI).

Active source rock

See Source rock.

American Petroleum Institute (API) gravity

A convenient scale of the American Petroleum Institute (API) that is inversely related to the density of liquid petroleum: API gravity = (141.5°/[specific gravity at 16°C] − 131.5°). A higher API indicates lighter oil. Fresh water has a gravity of 10° API. Heavy oils have less than 25° API, medium oils have 25 to 35° API, light oils have 35 to 45° API, and condensates have more than 45° API.

Asphaltenes

A complex mixture of heavy organic compounds in crude oils that precipitate under natural conditions due to the admixture of light hydrocarbons to the reservoir or in the laboratory by addition of excess n-pentane, n-hexane, or n-heptane. After precipitation of asphaltenes, the remaining oil consists of saturates, aromatics, and nitrogen, sulfur, and/or oxygen (NSO) compounds.

Backstripping

A key step in basin modeling, where successively older rock layers are removed to decompact underlying layers, thus allowing reconstruction of the burial history in a basin. The method requires decompaction of the remaining sequence of layers after each stage of backstripping to account for the amount of compaction at each step of burial.

Biodegradation

The microbial alteration of organic matter. Petroleum can undergo aerobic or anaerobic (e.g., sulfate-reducing or methanogenic) biodegradation during migration or while in the reservoir, or at surface seeps, typically at temperatures approximately less than 80°C (Haeseler et al., Section I; Guthrie et al., Section VI).

Bulk kinetics

A kinetic model where the generation of oil and gas from kerogen in the source rock is simulated using a single set of activation energies and frequency factors.

Burial history chart

A diagram that shows the depth of burial corrected for compaction of each rock unit (subsidence curve) versus the timing of the essential elements in a petroleum system, including the time interval and critical moment for petroleum generation. The calculated temperature history and the timing of petroleum generation based on calculated vitrinite reflectance or other maturity parameters are commonly overlain on the burial history diagram.

Calibration

A process where calculated model results are fit to measured data by adjusting key input parameters. For example, calculated present-day temperature and thermal maturity (e.g., vitrinite reflectance) at a given location within a sedimentary basin might be fit to measured temperatures and vitrinite reflectance values from a nearby well by adjusting paleoheat flow (Schenk et al., Section VI).

Capillary entry pressure

The pressure difference across the interface that separates two immiscible fluids, which is related to the force needed to move gas or a droplet of oil through a water wet pore. Capillary pressure increases for smaller pore diameters. The minimum capillary pressure measured in seal rock, such as shale, defines the maximum height of an oil or gas column that can be trapped beneath the seal, that is, the trap capacity.

Carrier bed

A permeable rock that conducts migrating petroleum.

Catagenesis

Thermal alteration of organic matter in the range of 50 to 150°C, typically requiring millions of years; equivalent to approximately 0.6 to 2.0% vitrinite reflectance.

Charge

The volume of petroleum expelled from the source rock that is available for entrapment.

Chromatography

Separation of mixtures of compounds based on physicochemical properties. Liquid chromatography and gas chromatography are used to separate petroleum compounds by retention time based on their tendency to partition between a mobile and stationary phase during movement through a chromatographic column.

Coal

A rock that contains greater than 50 wt. % organic matter. Most coals in North America and Europe originate mainly from higher plants and consist of type III (gas-prone) kerogen dominated by vitrinite group macerals. Thermal maturation transforms peat to lignite, bituminous coal, and then anthracite coal.

Common reflectance surface stack method

Common reflectance surface (CRS) sums more seismic traces and improves signal-to-noise ratio of subsurface images compared with classical common midpoint (CMP) stack methods of seismic analysis (Brink et al., Section II).

Condensate

Light oil with API gravity greater than 45°. The term was originally used for petroleum that is gaseous under reservoir conditions but liquid at surface temperatures and pressures.

Cracking

A thermal process where large molecules break apart into smaller molecules during burial maturation or in a refinery. Kerogen in source rocks and oil in reservoirs are cracked to generate lighter petroleum products at high temperatures.

Critical moment

The time that best depicts the generation-migration-accumulation of hydrocarbons in a petroleum system (Magoon and Dow, 1994). The geographic and stratigraphic extents of the system are best evaluated using a map and cross section drawn at the critical moment.

Crude oil

A natural mixture of hydrocarbons and other compounds that have not been refined. Produced crude oil commonly contains solution gas and closely resembles the original oil from the reservoir rock. Hydrocarbons are the most abundant compounds in crude oils, but they also contain nitrogen, sulfur, and/or oxygen (NSO) compounds and variable concentrations of trace elements, such as vanadium and nickel.

Darcy flow

A formula for single-phase fluid flow through porous media (Pegaz-Fiornet et al., Vayssaire, Section V).

Deasphalting

The process where asphaltenes precipitate from crude oil. Laboratory or refinery deasphalting is achieved by adding light hydrocarbons, such as pentane or hexane, to the oil. A similar process can occur in nature when methane and other light hydrocarbons that escape from deep reservoirs enter a shallower oil reservoir.

Decompaction

A burial history diagram requires that the present-day thickness of rock units be corrected to their original thickness before burial using a specific porosity-depth function for each lithologic unit. This involves sequential backstripping of each rock unit and restoration of the thickness of the immediately underlying unit before burial from the surface to basement until the entire sedimentary succession is restored to its original thickness.

Diagenesis

Chemical, physical, and biological changes that affect sediments during and after deposition and lithification but before oil generation or other significant changes caused by heat.

Discretization

The process of converting continuous features into discrete components. For example, various physical properties of each sedimentary unit in a basin model covering a large area, such as thermal conductivity or total organic carbon (TOC), can be divided into discrete values for each model cell, might measure 1 km wide × 1 km long × 400 m thick (0.6 mi × 0.6 mi × 1312 ft) (Wolf et al., Section IV).

Drilling mud

A mixture of clay, water, and chemicals that is pumped into and out of the borehole during drilling. Circulation of drilling mud cools the drill bit, flushes rock cuttings produced by the drill bit to the surface, and maintains pressure in the well bore.

Dry gas

Microbial or highly mature gas that is dominated by methane (>95% by volume) with little or no natural gas liquids. Microbial gas is depleted in ^{13}C compared with a highly mature gas.

Easy vitrinite reflectance (Easy% R_o)

An Arrhenius first-order kinetic model that uses a distribution of activation energies to calculate equivalent vitrinite reflectance (% R_o) for given time-temperature conditions (Sweeney and Burnham, 1990).

Effective source rock

See Source rock.

Essential elements

The source, reservoir, seal, and overburden rocks in a petroleum system (Magoon and Dow, 1994). The essential elements and the processes of generation-migration-accumulation and trap formation control the distribution of petroleum in the subsurface.

Events chart

A chart (also called timing-risk chart) that shows the timing of essential elements and processes for a petroleum system as well as the critical moment and the length of time required to preserve the accumulated petroleum until present day.

Expulsion

The process of primary migration where petroleum escapes from the source rock because of increased pressure and temperature. Expulsion generally involves short distances (meters to tens of meters).

First-order kinetics

See Kinetics.

Flowpath modeling

Simulation of instantaneous fluid flow through porous and permeable carrier beds as driven by buoyancy with essentially no resistance.

Frequency factor

A parameter in the Arrhenius equation that reflects reaction probability and is commonly expressed in geochemical kinetic modeling as s^{-1} or $m.y.^{-1}$. The frequency factor is also known as the A factor or, more rigorously, as the preexponential factor.

Gas hydrate

Various crystalline phases of water that contain gas (mainly methane) in arctic and deep-water settings.

Gas-prone

Organic matter that generates mainly hydrocarbon gases instead of oil during thermal maturation. Type III kerogen is gas prone.

Gas-to-oil ratio

The amount of hydrocarbon gas relative to oil in a reservoir, commonly measured in cubic feet per barrel.

Gas wetness

Expressed in various ways, but generally represents the amount of methane (C_1) relative to the total hydrocarbon gases ($C_1 + C_{2+}$) in a sample. For example, C_1/(C_1 to C_5) ratios greater than and less than 98% are dry and wet gases, respectively.

Generation-migration-accumulation

A petroleum system process that includes the generation, expulsion, and movement of petroleum from the pod of active source rock to the petroleum seep, show, or accumulation (Magoon and Dow, 1994).

Geographic extent

The area of occurrence of a petroleum system as defined by a line that encloses the pod of active source rock and all discovered shows, seeps, and petroleum accumulations that originated from that pod; the geographic extent is mapped at the critical moment (Magoon and Dow, 1994).

Geohistory diagram

See Burial history chart.

Geothermal gradient

The increase in temperature with depth in the Earth, commonly in degrees Celsius per kilometer or degrees Fahrenheit per 100 feet. Gradients are sensitive to basal heat flow, lithology, circulating groundwater, and the cooling effect of drilling fluids. Worldwide average geothermal gradients are from 24 to 41°C/km (1.3–2.2°F/100 ft), with extremes outside this range.

Gravity segregation

A process where heavier and lighter petroleum components accumulate near the bottom and top of the reservoir, respectively.

Heavy oil

Crude oil with less than 25° API.

Humic coal

Gas-prone (type III) coal that consists mainly of higher plant detritus, including vitrinite and inertinite group macerals, with little or no liptinite macerals.

Hydrogen index

A Rock-Eval pyrolysis measure of oil-generative potential defined as 100(S2/TOC) and measured in milligram hydrocarbons per gram total organic carbon (TOC). The HI is used on Van Krevelen–type plots of HI versus oxygen index (OI) to describe organic matter type, and a general relationship exists between HI and atomic hydrogen/carbon (H/C).

Hydrous pyrolysis

A laboratory technique where potential source rocks are heated without air, under pressure, and with water to artificially increase the level of thermal maturity.

Immature

Organic matter where conditions were too cool or too short in duration for thermal generation of petroleum, for example, vitrinite reflectance less than 0.6%.

Inactive source rock

See Source rock.

Inertinite

A maceral group composed of inert hydrogen-poor organic matter with little or no petroleum-generative potential. Type IV kerogen is dominated by inertinite.

Invasion percolation

Petroleum migration based on the distribution of capillary pressures in sediments and their evolution through time. Invasion percolation (IP) assumes instantaneous movement of petroleum under the effects of buoyancy and capillary pressure (Pegaz-Fiornet et al., Vayssaire, Section V).

Kerogen types I, II, IIS, III, IV

See Type.

Kinetics

Kinetic parameters that describe chemical reaction rates include the activation energy and frequency factor. Most petroleum system modeling assumes that oil and gas generation can be described by a series of parallel first-order kinetics, where the rate of each reaction depends on the concentration of only one reactant (a unimolecular reaction; Uguna et al., Schneider et al., Section I). See also Multicomponent kinetics.

Kitchen

See Pod of active source rock.

Level of certainty

A measure of the degree of confidence that petroleum originated from a specific pod of active source rock; three levels include known (!), hypothetical (.), and speculative (?), depending on the level of geochemical, geophysical, and geologic evidence (Magoon and Dow, 1994).

Light hydrocarbons

Gases and volatile liquids at standard temperature and pressure, which range from methane to octane, including normal, iso-, and cyclic alkanes, and aromatic compounds.

Light oil

Crude oil with 35 to 45° API.

Liptinite

A maceral group composed of oil-prone hydrogen-rich kerogen that fluoresces under ultraviolet light. Both structured (e.g., resinite, sporinite, or cutinite) and unstructured or amorphous liptinites, sometimes called amorphinite, can occur.

Maceral

Microscopically recognizable organic particles in kerogen. The three main maceral groups include liptinite, vitrinite, and inertinite.

Mantle

Part of the Earth composed mainly of solid silicate rock that extends from the base of the crust (Moho) to the core-mantle boundary at approximately 2900 km (~1802 mi) in depth.

Mature

Organic matter that is in the oil window; thermal maturity equivalent to the range of 0.6 to 1.4% vitrinite reflectance. Organic matter can also be mature with respect to the gas window (~0.9–2.0% vitrinite reflectance).

Maturity

See Thermal maturity.

McKenzie model

A mathematic expression for symmetrical tectonic rifting that assumes (1) an initial stretching phase with constant thinning of the crust and upper mantle caused by upwelling of the underlying asthenosphere (lower mantle) followed by (2) a cooling phase with near or full restoration of the thickness of the lithosphere (crust and upper mantle). The total thinning of the crust is described by a stretching factor, β.

Metagenesis

Thermal destruction of organic molecules by cracking to gas in the range approximately 150 to 200°C, which occurs after catagenesis, but before greenschist metamorphism (>200°C); thermal maturity equivalent to the range of 2.0 to 4.0% vitrinite reflectance.

Microbial gas

Also called marsh gas or biogenic gas; typically greater than 99% methane produced by methanogenic microbes in shallow sediments at temperatures less than 80°C. Microbial methane is generally depleted in ^{13}C compared with thermogenic gas.

Microscale sealed vessel pyrolysis (MSSV)

A laboratory heating procedure in the absence of air used to investigate the compositional variability of petroleum during increasing thermal maturation.

Migration

Movement of petroleum from source rock toward a reservoir or seep. Primary migration is expulsion of petroleum from fine-grained source rock, whereas secondary migration moves petroleum through a coarse-grained carrier bed or fault to a reservoir or seep. Tertiary migration occurs when petroleum moves from one trap to another or to a seep (Pegaz-Fiornet et al., Section V).

Mixing and upscaling

Single fluid or mineral properties can be used to derive bulk properties of mixtures, such as oil-wet limestone, by mathematically mixing the components in the same proportions thought to exist in nature. Arithmetic, harmonic, and geometric averaging are three methods used to mix components. Porosity is always arithmetically mixed, whereas grains (e.g., thermal conductivity) can be mixed geometrically for homogeneous sorting or arithmetically or harmonically for layered strata. Upscaling transforms microscale measurements, such as laboratory capillary entry pressure, to macroscale values that can be used in full-scale models. For example, capillary entry pressures for clastic and carbonate rocks can be estimated by dividing the laboratory measurements by an upscaling factor of 2.56 (Hantschel and Kauerauf, 2009).

Mohorovicic discontinuity

A zone that separates the Earth's crust from the underlying mantle (Brink et al., Section II). The Moho typically occurs approximately 35 km (~19 mi) below the continents and 5 to 10 km (3–5 mi) below the floor of the ocean.

Monte Carlo simulation

A set of model runs that requires the distribution of uncertainty for one or more variables, such as heat flow or thickness of a rock layer (see Uncertainty). Random values within the uncertainty distribution for each variable are used to derive the complete set of simulation results. Output parameters can be visualized and interpreted using statistical tools, such as histograms. Confidence intervals related to risking can be derived from these histograms, for example, "based on 1000 simulations, a 95% probability that this source rock generated at least 100 million barrels of petroleum exists."

Multicomponent kinetics

Kinetic models in which the generation of different subcomponents of the kerogen are individually simulated (i.e., each subcomponent has a different set of frequency factors and distribution of activation energies). These subcomponents can be defined by molecular weight range (e.g., C_7–C_{15}, C_{16}–C_{25}, C_{26}–C_{35}, C_{36}–C_{45}, C_{46}–C_{55}, C_{56}–C_{80}), compound type, or a combination thereof (Baur et al., Section VI).

Natural gas

Gaseous petroleum that can consist of C_1–C_5 hydrocarbons, CO_2, N_2, H_2, H_2S, Ar, and He. When natural gas occurs with oil, it is called associated gas.

Nitrogen, sulfur, and/or oxygen (NSO) compounds (resins)

The NSO compounds (resins) are pentane-soluble compounds in petroleum that contain various elements in addition to hydrogen and carbon, for example, nitrogen, sulfur, and/or oxygen (NSO). Compounds in this fraction are sometimes called heterocompounds or nonhydrocarbons. Other fractions include saturates, aromatics, and asphaltenes.

Nonassociated gas

Natural gas that is not associated with crude oil in the reservoir.

Nonhydrocarbon gases

Mainly carbon dioxide (CO_2), nitrogen (N_2), and hydrogen sulfide (H_2S), but also including helium (He), argon (Ar), and hydrogen (H_2).

Oil deadline

The depth where oil no longer exists as a liquid phase in petroleum reservoirs, generally corresponding to a gas-to-oil ratio (GOR) greater than 5000 SCF/barrel or more than 150°C (typically in the range 165–185°C).

Oil-oil correlation

A comparison of chemical compositions to describe the genetic relationships among crude oils based on source-related geochemical data such as biomarkers, isotopes, and metal distributions, although the source rock may not be defined.

Oil prone

Organic matter that generates significant quantities of oil during catagenesis. Oil-prone organic matter is typically also more gas prone than gas-prone organic matter.

Oil–source rock correlation

A comparison of chemical compositions to describe the genetic relationships among crude oils and source rock extracts based on source-related geochemical data such as biomarkers, isotopes, and metal distributions.

Oil window

The maturity range where oil is generated from oil-prone organic matter (~0.6–1.4% vitrinite reflectance), that is, within the catagenesis zone (~0.5–2.0% vitrinite reflectance).

Organic facies (organofacies)

A mappable rock unit that contains a distinctive assemblage of organic matter without regard to the mineralogy (Jones, 1987).

Organic matter

Biogenic carbonaceous materials. Organic matter preserved in rocks including kerogen, bitumen, pyrobitumen, oil, and gas.

Overburden rock

Sedimentary or other rock that compresses and contributes to the thermal maturation of the underlying source rock.

Overmature

See Postmature.

Oxygen index (OI)

A Rock-Eval pyrolysis measure of the amount of oxygen in organic matter defined as 100(S3/TOC) and measured in milligrams carbon dioxide per gram total organic carbon (TOC). The OI is used on Van Krevelen-type plots of hydrogen index (HI) versus OI to describe organic matter type, and a general relationship exists between OI and atomic oxygen/carbon (O/C).

Palynomorphs

Organic-walled acid-resistant microfossils that provide information on age, paleoenvironment, and thermal maturity (e.g., thermal alteration index [TAI]).

Permeability

The capacity of a rock layer to transmit water or other fluids, such as oil. The standard unit for permeability is the Darcy (d) or, more commonly, the millidarcy (md). Relative permeability is a dimensionless ratio that reflects the capability of oil, water, or gas to move through a formation compared with that of a single-phase fluid, commonly water. If a single fluid moves through rock, its relative permeability is 1.0. Two or more fluids generally inhibit flow through rock compared with that of a single phase of each component (Vayssaire, Section V).

Petroleum

A mixture of organic compounds composed mainly of hydrogen and carbon and found in the gaseous, liquid, or solid state in the Earth; includes hydrocarbon gases, bitumen, migrated oil, pyrobitumen, and their refined products, but not kerogen. In European usage, the term is sometimes restricted to refined products only.

Petroleum system

The essential elements (source, reservoir, seal, and overburden rock) and processes (trap formation, generation-migration-accumulation) and all genetically related petroleum that originated from one pod of active source rock and occurs in shows, seeps, or accumulations (Magoon and Dow, 1994); also called hydrocarbon system.

Petroleum system name

Systematic nomenclature (Magoon and Dow, 1994) that names (1) the formation containing the pod of active source rock followed by a hyphen, and (2) the reservoir rock that contains the largest volume of genetically related petroleum, followed by (3) a symbol for the level of certainty in the petroleum system, for example, Bazhenov-Neocomian(!)

Petroleum system processes

Trap formation and generation-migration-accumulation. Biodegradation and thermal destruction are omitted as processes because they occur after a petroleum system forms.

PhaseKinetics

A method based on pyrolysis experiments to determine compositional kinetic models that allows prediction of petroleum-phase properties and behavior during thermal modeling (di Primio and Horsfield, 2006).

Phytoclast

An identifiable particle or maceral in kerogen, for example, phytoclasts of vitrinite are used to measure vitrinite reflectance.

Pod of active source rock

A contiguous volume of fine-grained organic-rich rock that generated and expelled petroleum at the critical moment. A pod of thermally mature source rock may be active, inactive, or spent.

Porosity

The volume percent of a rock that consists of open pore space.

Postmature (for oil)

High maturity at which no further oil generation occurs (i.e., >1.3% vitrinite reflectance).

Potential source rock

See Source rock.

Primary migration

See Expulsion or Migration.

Production index

A Rock-Eval pyrolysis measure of thermal maturity or contamination measured as S1/(S1 + S2).

Pseudo–Van Krevelen diagram

See Van Krevelen diagram.

Pyrolysis

Breakdown of organic matter by heating in the absence of oxygen; Rock-Eval instrumentation uses programmed-temperature pyrolysis because the temperature is programmed to increase at a selected rate during analysis (25°C/min). Hydrous pyrolysis uses a constant temperature for each experiment (e.g., 330°C).

Ray tracing

A migration approach that assumes petroleum migrates instantaneously under the influence of buoyancy through a fault network or porous carrier bed.

Relative permeability

See Permeability.

Reservoir

A porous and permeable sedimentary rock formation that contains oil and/or natural gas enclosed or surrounded by layers of less permeable rock. An oil pool consists of a reservoir or group of reservoirs. However, the term is misleading because petroleum does not exist in pools, but in pores between rock grains.

Reservoir characterization

Integrating and interpreting geologic, geophysical, petrophysical, fluid and performance data to describe a reservoir.

Reservoir rock

Porous and permeable rock, such as sandstone, vuggy carbonate, or fractured shale, that permits migration and accumulation of petroleum provided that an overlying or updip trap is present.

R_o

See Vitrinite reflectance.

Rock-Eval

A commercially available pyrolysis system used as a rapid screening tool to evaluate the quantity, quality, and thermal maturity of rock samples.

S1, S2, S3

Rock-Eval pyrolysis parameters where S1 = volatile organic compounds (mg hydrocarbons/g rock); S2 = organic compounds generated by cracking of the kerogen (mg hydrocarbons/g rock); and S3 = organic carbon dioxide generated from the kerogen up to 390°C (mg CO_2/g rock).

Seal rock (cap rock)

Fine-grained rock that is relatively impermeable to migrating petroleum in the subsurface, such as shale or anhydrite, thus slowing or preventing leakage of petroleum to the surface.

Secondary migration

See Migration.

Solid bitumen

Solid bitumen includes pyrobitumen and bitumen formed by nonthermal processes, such as deasphalting or biodegradation (Derks et al., Section IV).

Source rock

Rock that contains sufficient organic matter of the proper composition to generate and expel petroleum during diagenesis (microbial methane) or catagenesis. Source rock can be effective (is generating or has generated and expelled), potential (sufficient quantity and quality of organic matter, but has not yet expelled), active (is generating and expelling petroleum at the critical moment), inactive (stopped generating because of uplift and/or reduced thermal stress, although petroleum potential remains), or spent (postmature for oil but can still generate methane and wet gas).

Spent source rock

See Source rock.

Standard temperature and pressure (STP)

Defined as room temperature (15.6°C or 60°F) and one atmosphere pressure (14.7 psi).

Suboxic

Refers to water column or sediments with molecular oxygen contents of 0 to 0.2 mL/L of interstitial water.

Subsidence curve

See Burial history chart.

Tectonic inversion

A process where extensional normal faults are reactivated by compression (positive inversion), or where reverse faults are reactivated by extension (negative inversion). Positive inversion results in uplift of formerly low-lying areas (Nelskampe et al., Section III).

Tertiary migration

See Migration.

Thermal maturity

The extent of heat-driven reactions that alter the composition of organic matter (e.g., conversion of sedimentary organic matter to petroleum or cracking of oil to gas). Different geochemical scales, such as vitrinite reflectance, pyrolysis T_{max}, and biomarker maturity ratios can be used to indicate the level of thermal maturity of organic matter.

Total organic carbon (TOC)

Total organic carbon ([TOC] wt. %) in a rock sample as determined by various combustion methods.

Transformation ratio

Ranges from 0 to 1.0 and is the ratio of the generated petroleum to the original petroleum potential of a sample before maturation (Derks et al., Section IV).

Trap

A subsurface arrangement of relatively impermeable rock that allows accumulation of petroleum in underlying or downdip, relatively porous, reservoir rock. Traps can be structural (e.g., domes, anticlines), stratigraphic (pinch-outs, permeability or diagenetic changes), or combinations of both.

Type I kerogen

Highly oil-prone organic matter having Rock-Eval pyrolysis hydrogen indices greater than 600 mg hydrocarbon/g TOC when thermally immature; contains algal and bacterial input dominated by amorphous liptinite macerals; common in both marine and lacustrine settings; type I pathway on Van Krevelen diagram.

Type II kerogen

Oil-prone organic matter having Rock-Eval pyrolysis hydrogen indices in the range of 300 to 600 mg hydrocarbon/g TOC when thermally immature; contains algal and bacterial organic matter dominated by liptinite macerals, such as exinite and sporinite; common but not restricted to marine settings; Type II pathway on Van Krevelen diagram.

Type IIS kerogen

Hydrogen indices in the range of type II kerogen, but sulfur-rich type IIS kerogens contain uncommonly high organic sulfur (8–14 wt. %, atomic $S/C \geq 0.04$) and begin to generate oil at a lower thermal maturity than typical type II kerogens with less than 6 wt. % sulfur (Orr, 1986).

Type III kerogen

Gas-prone organic matter having Rock-Eval pyrolysis hydrogen indices in the range of 50 to 200 mg hydrocarbon/g TOC when thermally immature; generally contains higher plant organic matter dominated by vitrinite macerals, common but not restricted to paralic marine settings, type III pathway on Van Krevelen diagram.

Type IV kerogen

Inert organic matter having Rock-Eval pyrolysis hydrogen indices below 50 mg hydrocarbon/g TOC in thermally immature rocks; dominated by organic matter that was recycled or extensively oxidized during deposition. Sometimes the type IV pathway is not shown on Van Krevelen diagrams, but it lies below the type III pathway.

Uncertainty

The possible distribution of values for one number, such as the thermal conductivity of shale. Uncertainty distributions must be specified for Monte Carlo simulations, for example, normal (Gaussian), logarithmic normal, uniform, triangular, or exponential (Hicks et al., Schoellkopf et al., Section V).

Uniform stretching model

See McKenzie model.

Upscaling

See Mixing and upscaling.

Van Krevelen diagram

A plot of atomic oxygen/carbon (O/C) versus atomic hydrogen/carbon (H/C) originally used to classify coals and predict compositional evolution during thermal maturation, but adapted to classify kerogen types I, II, III, and IV. More common is the pseudo–Van Krevelen diagram, where Rock-Eval pyrolysis oxygen index ([OI] mg HC/g TOC) is plotted versus hydrogen index ([HI] mg HC/g TOC).

Viscosity

Fluid viscosity is a measure of the resistance of a fluid to flow. The viscosity of liquid oil depends on its composition, temperature, and pressure.

Vitrinite

A group of gas-prone macerals derived from land plant tissues. Phytoclasts of vitrinite are used for vitrinite reflectance (R_o) determination of thermal maturity.

Vitrinite reflectance (R_o)

A thermal maturation parameter based on microscopy of organic matter in fine-grained rocks. Each R_o value represents the percent of incident light (546 nm) reflected from a single vitrinite phytoclast in a polished slide of kerogen, coal, or whole rock under an oil-immersion microscope objective as measured by a photometer. Average R_o is typically measured on at least 20 randomly oriented vitrinite phytoclasts. Some microscopes have rotating stages that allow measurements of anisotropy. Thus, R_m, R_{max}, R_{min}, and R_r indicate mean, maximum, minimum, and random vitrinite reflectance, respectively.

Wet gas

Natural gas that contains ethane, propane, and heavier hydrocarbons and less than 98% methane/total hydrocarbons. The wet gas zone occurs during catagenesis below the bottom of the oil window and above the top of the gas window (1.4–2.0% vitrinite reflectance).

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APPENDIX

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2. First stoichiometric model of oil biodegradation in natural petroleum systems. Part II: Application of the BioClass 0D approach to oils from various sources by F. Haeseler, F. Behar, and D. Garnier
3. Model of low-maturity generation of hydrocarbons applied to the Carupano Basin, offshore Venezuela by F. J. Schneider, J. Noya, and C. Magnier

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11. A new efficient scheme to model hydrocarbon migration at basin scale: A pressure-saturation splitting by S. Wolf, I. Faille, S. Pegaz-Fiornet, F. Willien, and B. Carpentier

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18. Petroleum system modeling of northern Alaska by O. Schenk, K. J. Bird, L. B. Magoon, and K. E. Peters

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