Fundamentals of Basin and Petroleum Systems Modeling

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Preface

It is with great satisfaction and personal delight that I can write the foreword for this book *Fundamentals of Basin and Petroleum Systems Modeling* by Thomas Hantschel and Armin Ingo Kauerauf. It is a privilege for us geoscientists that two outstanding physicists, with scientific backgrounds in numerical methods of continuum-mechanics and in statistical physics respectively could be won to deeply dive into the numerical simulation of complex geoprocesses. The keen interest in the geosciences of Thomas Hantschel and Armin I. Kauerauf and their patience with more descriptive oriented geologists, geochemists, sedimentologists and structural geologists made it possible to write this book, a profound and quantitative treatment of the mathematical and physical aspects of very complex geoprocesses. In addition to their investigative interest during their patient dialogue with afore mentioned geological specialists Thomas Hantschel and Armin I. Kauerauf gained a great wealth of practical experience by cooperating closely with the international upstream petroleum industry during their years with the service company IES, Integrated Exploration Systems. Their book will be a milestone in the advancement of modern geosciences.

The scientific and the practical value of modern geosciences rests to a large degree upon the recognition of the complex interrelationship of individual processes, such as compaction, heat-, fluid- and mass-flow, reaction kinetics etc. and upon the sequential quantification of the entire process chain. The intelligent usage of modern high speed computers made all this possible.

Basin modeling was for many years considered as "a niche discipline", mainly propagated and used by geochemists. What a fundamental error and misunderstanding! The absolute contrary is the truth. Basin modeling integrates practically all geoscientific disciplines, it allows an unprecedented quantitative understanding of entire process chains and it detects quickly inconsistencies or uncertainties in our knowledge base. In short, the basin modeling–approach is a big step forward in modern geosciences. This book is a challenge for academic teachers in the geosciences and likewise for scientists and engineers in the petroleum and mining industry. The challenge is to educate much more than in the past the younger ones among us to be able to walk along the borderline between the exact sciences with a physcial and mathematical background and the classical geosciences and vice versa.

In 1984 Prof. Bernard Tissot and I wrote in the Preface of the second edition of our book *Petroleum Formation and Occurrence*: “It is evident that computer modeling is here to stay, and may very well revolutionize the field. The computer can be used as an experimental tool to test geological ideas and hypotheses whenever it is possible to provide adequate software for normally very complicated geological processes. The enormous advantages offered by computer simulation of geological processes are that no physical or physico-chemical principles are violated and that for the first time the geological time factor, always measured in millions of years rather than in decades, can be handled with high speed computers with large memories. Thus, the age of true quantification in the geosciences has arrived. We believe that this computer-aided, quantitative approach will have an economic and intellectual impact on the petroleum industry, mainly on exploration.” All this indeed is the case now. And even more so, basin modeling enhances and deepens the intelligent interpretation of geological data acquired by geophysical, geological and geochemical methods and thus converts static information into dynamic process understanding.

I congratulate the two authors for their excellent textbook. I urge the geoscientific community to dig into the wealth of scientific information offered in this book. It will help us to understand and quantify the dynamics occurring in the subsurface.

Dietrich Welte

In the late 1970s “Basin Modeling” was introduced as the term describing the quantitative modeling of geological processes in sedimentary basins on geological timescales. At that time basin models found their main application in heat and pore water flow modeling with regard to sediment compaction and temperature controlled chemistry of hydrocarbon generation. Since then geological, chemical, and transport related models have much improved. Basin modeling turned into a complex and integrated framework of many processes, such as multiphase fluid flow for hydrocarbon migration and accumulation, advanced reaction schemes for organic and mineral transformations or compressional and extensional tectonics.

The term “Basin Modeling” is not only used for the modeling of processes in sediments, but also for the modeling of crustal and mantle heat and mass flow processes to predict the sedimentary basin type and the related tectonic subsidence. We prefer the naming “Crustal Models”’ for this type of analysis. Obviously, processes in the crust are tightly linked to the sedimentary basin and hence integrated basin and crustal models have also been developed.

In addition to pure scientific research there has always been a commercial motivation for basin modeling as a means to understand, quantify and predict petroleum repositories. From the start, the petroleum industry has been the main sponsor for the development of basin modeling tools for exploration and resource assessment. Over time, a number of specialized tools and different types of basin modeling simulators have been developed and with them new terminologies have been introduced, such as “Petroleum Systems Modeling”, “Exploration Risk Assessment” or “Prospect and Play Analysis”.

We, the authors of this book, are both physicists with a focus on numerical modeling and software design. Since 1990 and 1997 respectively, we have developed major parts of various generations of the commercial basin simulation software PetroMod®. Furthermore, we have offered many training courses on the subject of the theory and fundamental principles behind basin modeling. The training courses contain a fair amount of mathematics, physics and chemistry – the basic building blocks of the software tools. A complete simulation of an actual geological basin often displays complex fluid flow and accumulation patterns which are difficult to interpret. We believe that a basic understanding of the theory behind the tools is essential to master the models in detail.

Most basin modelers, in scientific research institutions or the petroleum industry, are expert geologists, coming from an entirely different academic domain. They may therefore be unfamiliar with the mathematics and quantitative science related to the software. This results in an abundance of excellent literature about basin modeling from the geological point of view but no comprehensive study regarding mathematics, physics and computer science.

The book is intended above all as an introduction to the mathematical and physical backgrounds of basin modeling for geologists and petroleum explorationists. Simultaneously, it should also provide (geo)physicists, mathematicians and computer scientists with a more in–depth view of the theory behind the models. It is a challenge when writing for an interdisciplinary audience to find the balance between the depth and detail of information on the one hand and the various educational backgrounds of the readers on the other. It is not mandatory to understand all of the details to comprehend the basic principles. We hope this book will be useful for all parties.

With this work we also wanted to create a handbook offering a broad picture of the topic, including comprehensive lists of default values for most parameters, such as rock and fluid properties and geochemical kinetics. We hope that our compilation will ease the work of many modelers. The book is not intended as an introduction to the geological principles of basin formation nor as a tutorial to practical basin modeling. Case studies have not been included. A second volume focusing on case studies and the practical aspects of the application is planned for the future.

Experts in sedimentology, petrology, diagenesis, fault seal analysis, fracturing, rock mechanics, numerics, and statistics may find the approach to some topics in this book too simplistic, but we deliberately came to the decision to open the book to a broader interdisciplinary understanding. At the same time we also feel that we present in many instances ideas which could inspire further studies.

The main focus has been on numerical models and features. Naturally, there is a tendency to focus on features which we ourselves developed for PetroMod®, but most of the basic models are also applicable for other academic and commercial software programs. Since there are not many publications by other development groups about the fundamentals, theory and parameters of their work, we were often unable to include appropriate references in our discussion.

Basin modeling is a multi–disciplinary science. We hope that students, researchers and petroleum explorers with very different experiences will benefit from the presented work.

Acknowledgments

We wish to acknowledge our families who tolerated many long hours on the computer, in the evening and at the weekend.

IES, which recently became part of Schlumberger, was very generous in supporting this work. It is hardly conceivable for us to write such a book without the infrastructure, support and friendly atmosphere at IES.

We appreciate the IES geologists, who tried to teach us basics about geology and supplied us continuously with test models and data. Many examples in this volume can be attributed to their work.

Special thanks go to the IES software development team, which provided us among others with excellent software for building and analyzing basin models.

We are indebted to Thomas Fuchs, Michael de Lind van Wijngaarden and Michael Fücker for many interesting discussions. Our understanding was again and again improved, in general and in detail.

It must be pointed out, that many rock data values and correlations which were not published up to now are originally from Doug Waples. He did a great job of collecting data over many years.

Special acknowledgments are due to the patient referees Michael Hertle, Bernd Krooss, Tim Matava, Ken Peters, Øyvind Sylta, René Thomson, Doug Waples, Dietrich Welte, Michael de Lind van Wijngaarden, Bjorn Wygrala and Gareth Yardley. Hopefully, we did not stress them too much.

Chris Bendall and Katrin Fraenzel checked spelling and grammar. Thanks for the hard job.

Finally we should gratefully mention all colleagues, customers and friends who accompanied us during the last years. We wanted to avoid missing a person, so we abdicated a huge list.

Further special acknowledgments from Armin are due Dr. Gerich–Düsseldorf, Dr. Kasparek and Dr. Schäfer who diagnosed a serious disease in April 2008. Prof. Dr. Autschbach and his team at the RWTH–Klinikum were able to save Armin's life in an emergency surgery. Many thanks. Unfortunately, this delayed the appearance of the book at least for two additional months and we have a suitable justification for some typos.

December, 2008 Thomas Hantschel and Armin I. Kauerauf

Contents

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Introduction to Basin Modeling

1.1 History

Geology and geochemistry in sedimentary basins have been established sciences for centuries. Important textbooks, such as Tissot and Welte (1984); Hunt (1996); Gluyas and Swarbrick (2004); Peters et al. (2005); Allen and Allen (2005), summarize the knowledge especially related to petroleum geosciences.

The first basin modeling computer programs were developed around 1980 (Yükler et al., 1979). The main concept encompassed multi–1D heat flow simulation and subsequent geochemical models to construct petroleum generation and expulsion maps for the evaluation of source rock maturity. One of the key tasks was to calculate and calibrate the temperature history during the evolution of a geological basin. Heat flow calculation is one of the best investigated problems in applied engineering. A formulation and solution of the corresponding differential equations can be easily achieved. Once the paleo–temperatures were known, equations for chemical kinetics could be used to evaluate the cracking rates of petroleum generation. Another important part of the analysis was the prediction of pore fluid pressures. Transport equations for one fluid phase with a special term for the overburden sedimentation rate were used to calculate the compaction of the sediments. The compaction state and related porosity facilitated the determination of bulk thermal conductivities for heat flow calculations. At that time, practical studies were mainly performed as 1D simulations along wells, because the computer capabilities were still limited and multiphase fluid flow for migration and accumulation of petroleum had not been well implemented. Temperature profiles from multi–well analysis were used to calculate petroleum generation with source rock maturity maps over time and the determination of the peak phases of oil and gas expulsion. This concept is still used when data are scarce in early exploration or when the project requires some quick output.

From 1990 to 1998 a new generation of basin modeling programs became the standard in the petroleum industry. The most important new feature was

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the implementation of refined fluid flow models with three phases: water, liquid petroleum, and gas. In commercial packages, 2D Darcy flow models and map based flowpath analysis were realized (Ungerer et al., 1990; Hermanrud, 1993). Darcy flow models are able to model all relevant processes of flow, accumulation, and seal break through. They are based on differential equation systems for the competing fluid phases. However, they are restricted to 2D simulators, since they require a high computing and development effort. The map based flowpath technique redistributes pre-calculated expulsion amounts of petroleum along reservoir–seal interfaces within the reservoirs. Accumulation bodies are calculated under correct conservation of the petroleum mass and volume. The approach is based on some crude approximations concerning flow. However, it considers horizontal spilling from one drainage area to the next and simple break through when the column pressure exceeds the seal capability. Most models under study were first performed in 2D along cross sections because pre-interpreted horizons and faults along 2D seismic lines were readily available. Calculated generation and expulsion amounts were again used for the flowpath analysis afterwards. Although 2D Darcy flow models work very well, they were rarely used in practical exploration studies as horizontal petroleum migration in the third dimension can not be neglected. Another important innovation was the implementation of special geological processes such as salt dome tectonics, refined fault behavior, diffusion, cementation, fracturing, and igneous intrusions.

In 1998, a new generation of modeling programs were released changing the workflow of most basin modeling studies once again. Many new features were related to petroleum migration and the characteristics of reservoirs. Most programs and tools focused on 3D functions with improved features for model building and increased simulator performance. From that time on, most of the heat and pore pressure calculations were performed in full 3D. This required the interpretation and mapping of a relatively complete set of horizons instead of just the horizons of the reservoirs. Three–phase–Darcy flow models were also made available in 3D. However, high computation efforts were necessary while simplifying the model's premises to a large degree. Consequently the model's resolution was restricted which often led to unrealistic or oversimplified geometries. Pure Darcy flow models were not applicable in practice. Three alternatives for modeling migration were developed. One was the use of the well established flowpath models, the other two are new developments: hybrid flow simulators and the invasion percolation method. Hybrid fluid flow models use domain decomposition to solve the Darcy flow equations only in areas with low permeabilities and flowpath methods in areas with high permeabilities, resulting in a significant decrease of computing time. Invasion percolation is another rule based transport technique which focuses on capillary pressure and buoyancy without any permeability controlled flow timing. Another new feature was the implementation of multicomponent resolved petroleum phases and the development of fast thermodynamic PVT (Pressure Volume Temperature) controlled fluid analysis based on flash calculation for these components. Between four and fourteen fluid components (chemical species) are usually taken into consideration, replacing the traditional two component (oil–gas) black oil models. Reservoir composition and petroleum quality prediction were significantly improved. Simultaneously, better computer hardware especially PC clusters combined with parallelized simulators, reduced computing times significantly. Furthermore, statistics for calibration, risk analysis for quantification of probability for success or failure and the consideration of extensional and compressional tectonics significantly increased the applicability of basin modeling. Integrated exploration workflows, which incorporate basin modeling, became a standard in the industry.

1.2 Geological Processes

Basin modeling is dynamic modeling of geological processes in sedimentary basins over geological time spans. A basin model is simulated forward through geological time starting with the sedimentation of the oldest layer until the entire sequence of layers has been deposited and present day is reached. Several geological processes are calculated and updated at each time step (Fig. 1.1). Most important are deposition, compaction, heat flow analysis, petroleum generation, expulsion, phase dissolution, migration, and accumulation.

Deposition

Layers are created on the upper surface during sedimentation or removed during erosion. It is assumed that the geological events of deposition and hiatus are known. Therefore, paleo times of deposition can be assigned to the layers.

The depositional thickness of a new layer is calculated via porosity controlled backstripping from present day thickness or imported from structural restoration programs. The overall geometry may also change due to salt movement or magmatic intrusions. Estimated backstripping amounts yield calculated present day thicknesses which are not identical with the given present day geometry. The differences facilitate a better estimation of the depositional thicknesses in the next simulation run. This method of organizing multiple forward simulations to calibrate against the present day geometry is referred to as optimization procedure.

Pressure Calculation and Compaction

Pressure calculation is mainly a one–phase water flow problem which is driven by changes of the overburden weight due to sedimentation. Additionally, internal pressure building processes such as gas generation, quartz cementation and mineral conversions can be taken into account.

Pore pressure reduction entails compaction and leads to corresponding changes in the geometry of the basin. That is why pressure calculation and compaction have to be performed before heat flow analysis in each time step.

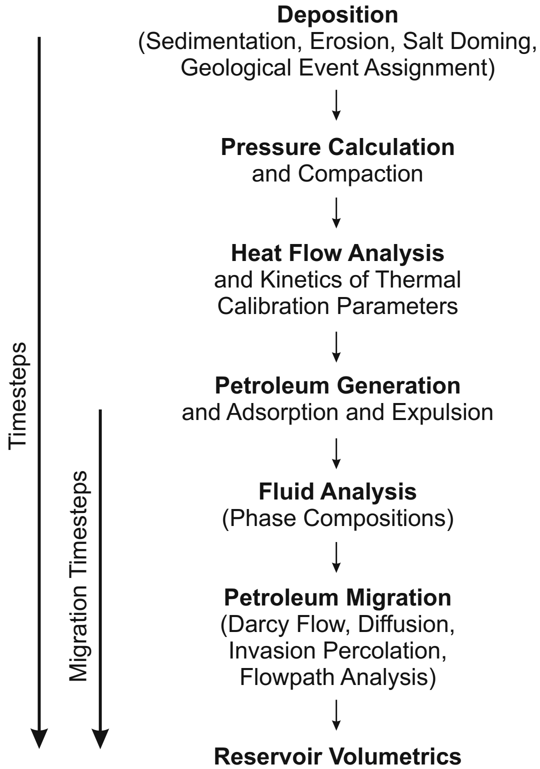

Fig. 1.1. Major geological processes in basin modeling

Heat Flow Analysis

Temperature calculation is the target of the heat flow analysis. It is a necessary prerequisite for the determination of geochemical reaction rates. Heat conduction and convection as well as heat generation by radioactive decay must be taken into consideration. Igneous intrusions require the inclusion of thermal phase transitions in sediments. Thermal boundary conditions with inflow of heat at the base of the sediments must be formulated. These basal heat flow values are often predicted with crustal models in separate preprocessing programs or are interactively calculated for each geological event.

Kinetics of Calibration Parameters

It is possible to predict vitrinite reflectance values, the concentration of molecular biomarkers and apatite fission tracks with suitable models which are based on Arrhenius type reaction rates and simple conversion equations. These predictions are temperature sensitive and can therefore be compared to measured data so that uncertain thermal input data, such as paleo–heat flow values, can be restricted or even calibrated.

Petroleum Generation

The generation of petroleum components from kerogen (primary cracking) and the secondary cracking of the petroleum is usually described with sets of parallel reactions of decomposition kinetics. The number of chemical components vary between two (oil, gas) and twenty. The cracking schemes can be quite complex when many components and secondary cracking are taken into account. Adsorption models describe the release of hydrocarbons into free pore space of the source rock.

Fluid Analysis

The generated hydrocarbon amounts are mixtures of chemical components. Fluid flow models deal with fluid phases which are typically liquid, vapor and supercritical or undersaturated phases. Therefore temperature and pressure dependent dissolution of components into the fluid phases is studied during fluid analysis. The two most important fluid models are the rather simple black oil model and the thermodynamically founded multicomponent flash calculations. Fluid phase properties, such as densities and viscosities, are also derived from fluid models. They are essential for accurate migration modeling and reservoir volumetrics.

Darcy Flow and Diffusion

Darcy flow describes multicomponent three phase flow based on the relative permeability and capillary pressure concept. It can be applied for migration. Migration velocities and accumulation saturations are calculated in one procedure. Special algorithms are used to describe break through and migration across or in faults. Diffusion effects can be evaluated for the transport of light hydrocarbons in the water phase.

Flowpath Analysis

In carriers lateral petroleum flow occurs instantaneously on geological timescales. It can be modeled with geometrically constructed flowpaths. Information about drainage areas and accumulations with compositional information can easily be obtained. Spilling between and merging of drainage areas must be taken into account. Flowpath analysis in combination with Darcy flow in low permeability regions is called the hybrid method. Migration modeling without sophisticated Darcy flow, instead using simplified vertical transport of generated hydrocarbons into carriers, is commonly called flowpath modeling.

Invasion Percolation

Migration and accumulation can alternatively be modeled with invasion percolation. This assumes that on geological timescales petroleum moves instantaneously through the basin driven by buoyancy and capillary pressure. Any time control is neglected and the petroleum volume is subdivided into very small finite amounts. Invasion percolation is very convenient to model in–fault flow. The method is especially efficient for one phase flow with the phase consisting of only a few hydrocarbon components.

Reservoir Volumetrics

The column height of an accumulation is balanced by the capillary entry pressure of the corresponding seal. Leakage and break through are therefore important processes reducing the trapped volume. Other processes such as secondary cracking or biodegradation also have a serious impact on the quality and quantity of the accumulated volume.

In principle all processes depend on each other. Therefore, at a given time, all these coupled processes must be solved together with the solution of the last time step as the initial condition. For numerical reasons such an approach can be performed implicitly in time and is thus called an implicit scheme. In practice it is found, that the processes can be decoupled, very often to some high order of accuracy. Finally it is possible to solve for all the processes which are shown in Fig. 1.1 in the given order. Extra loops with iterative updates for higher accuracy can easily be performed. Decoupled schemes are often called explicit schemes, especially if the processes itself are treated explicitly in time.

For example, migration and accumulation seldom has an important effect on basin wide compaction. Thus migration can often be treated independently. However, a coupling of migration with compaction might arise with pressure updates due to gas generation and subsequent local modification of the geometry. By re-running the entire simulation with consideration of the gas pressure of the previous run, the modified geometry can in principle be iteratively improved until convergence is reached. In practice, it is often found, that only very few iterative runs are necessary.

For the implicit scheme, the temporal evolution of the basin must obviously be calculated on the smallest timescale of all involved geological processes. A big advantage of an explicit scheme is the fact, that each explicitly treated process can be solved on its own timescale. On the other hand, time steps of implicitly treated processes can often, for numerical reasons, be longer than time steps of explicitly treated processes. This increases the performance of the implicit scheme, especially when iterative feedback loops have to be taken into account in explicit schemes. In practice, a combination of both schemes is found to be most advantageous. This yields three types of time steps, which are often called events, basic and migration time steps.

The outer time loops are identical with geological events. They characterize the period in which one layer has been uniformly deposited or eroded or when a geological hiatus occurred. Thus, the total number of events is almost equal to the number of geological layers and usually ranges between 20 and 50. Events are subdivided into basic time steps with one solution for pressure or compaction and the heat equations. The length of the basic time step depends on deposition or erosion amounts and on the total duration of the event. The total number of time steps usually lies between 200 and 500. The basic time steps are further subdivided into migration steps for an explicitly treated Darcy flow analysis. In one migration time step the transported fluid amount per cell is usually restricted to the pore volume of that cell. Therefore the total number ranges from 1000 up to 50000 and more and depends on the flow activity and the selected migration modeling method. All time loops for events, basic time steps and migration time steps are commonly managed automatically in most simulators. Mathematical convergence is often ensured by empirical rules for step length calculation.

Transport Processes

Heat flow, pore pressure and compaction, Darcy flow migration processes, and diffusion are transport processes. They follow a similar scheme of description, derivation, and formulation of the basic equations. The core problem is the interaction of two basic quantities, the state and the flow variable (Table 1.1). The influence of a flow variable acting from any location on any other neighboring location is the main part of the mathematical formulation. Modeling of transport problems requires a major computing effort.

For example, temperature and heat flow are the corresponding basic variables for heat conduction. Temperature is the state variable and heat flow is the corresponding flow variable. A temperature difference (or gradient) causes a heat flow, and the heat flow decreases the temperature difference. The heat flow is controlled by the thermal conductivity and the temperature response by the heat capacity.

State variable	Flow variable	Flow equation	Material property
Temperature T	Heat flow $\mathbf{q}$	$\mathbf{q} = -\boldsymbol{\lambda} \cdot \operatorname{grad} T$	Thermal conductivity $\boldsymbol{\lambda}$
Pressure p	Water flow $\mathbf{v}_w$	$\mathbf{v}_w = -\dfrac{\mathbf{k}}{\nu} \cdot \operatorname{grad}(p - \rho g z)$	Permeability $\mathbf{k}$ and viscosity ν
Fluid potential u_p	Fluid flow $\mathbf{v}_p$	$\mathbf{v}_p = -\dfrac{\mathbf{k}k_{rp}}{\nu_p} \cdot \operatorname{grad} u_p$	Relative perm. $\mathbf{k}k_{rp}$ and viscosities ν_p
Concentration c	Diffusion flux $\mathbf{J}$	$\mathbf{J} = -D \operatorname{grad} c$	Diffusion coeff. D

Table 1.1. Fundamental physical transport laws and variables

In general, an energy or mass balance can be used to formulate a boundary value problem with appropriate boundary conditions and to calculate the development of both the state and the flow variables through geological time. A solution to the boundary value problem requires in practice a discretization of the basin into cells and the construction and inversion of a large matrix. The matrix elements represent the change of the state variable caused by the flow between two neighboring cells. The number of cells is the number of unknowns. Finally, an inversion of the matrix results in the solution vector, e.g. containing a temperature inside of each cell.

The inversion of transport processes is often the major computing effort in basin modeling (Chap. 8). It depends strongly, almost exponentially, on the number of cells and therefore the resolution.

Examples of non-transport processes are fluid analysis, chemical kinetics and accumulation analysis, which depend only linearly on the number of cells if they are separated and explicitly treated. These processes can then be modeled very efficiently.

1.3 Structure of a Model

The general analysis of the basin type and the main phases of basin evolution precede the construction of the model input data. This encompasses information about plate tectonics, rifting events, location of the basin, and depositional environments through geological time, global climates, paleo–bathymetries, and tectonic events. The model input is summarized in Fig. 1.2, and includes: present day model data with depth horizons, facies maps, fault planes, the age assignment table for the geological event definition, additional data for the description of paleo–geometries, thermal and mechanical boundary conditions through geologic time, the property values for lithologies, fluids, and chemical kinetics.

1 **Present Day Model**
- Horizons (Depth/Structure Maps)
- Facies Maps
- Fault Surfaces

2 **Age Assignment**

3 **Paleo Geometry**
- Water Depth Maps
- Erosion Maps
- Salt Thickness Maps
- Paleo Thickness Maps

4 **Boundary Conditions**
- SWI-Temperature Maps
- Basal Heat Flow Maps

5 **Facies**
- Facies Definitions
- TOC & HI Maps
- Rock Composition Maps

6 **Seismic** (optional)
- Attributes (Cubes, Maps)
- Reference Horizons for Depth Conversion

Fig. 1.2. Basic elements of model input

Present Day Model Data

A sedimentary basin is a sequence of geological layers. Each of the layers contains all the particles which have been deposited during a stratigraphic event. A horizon is the interface between two layers (Fig. 1.3) and usually interpreted from a seismic reflection surface. Seismic interpretation maps and lines (in 2D) are usually not extended over the entire model area and have to be inter– and extrapolated and calibrated with well data. The construction of the horizon stacks often requires most of the time for the model building.

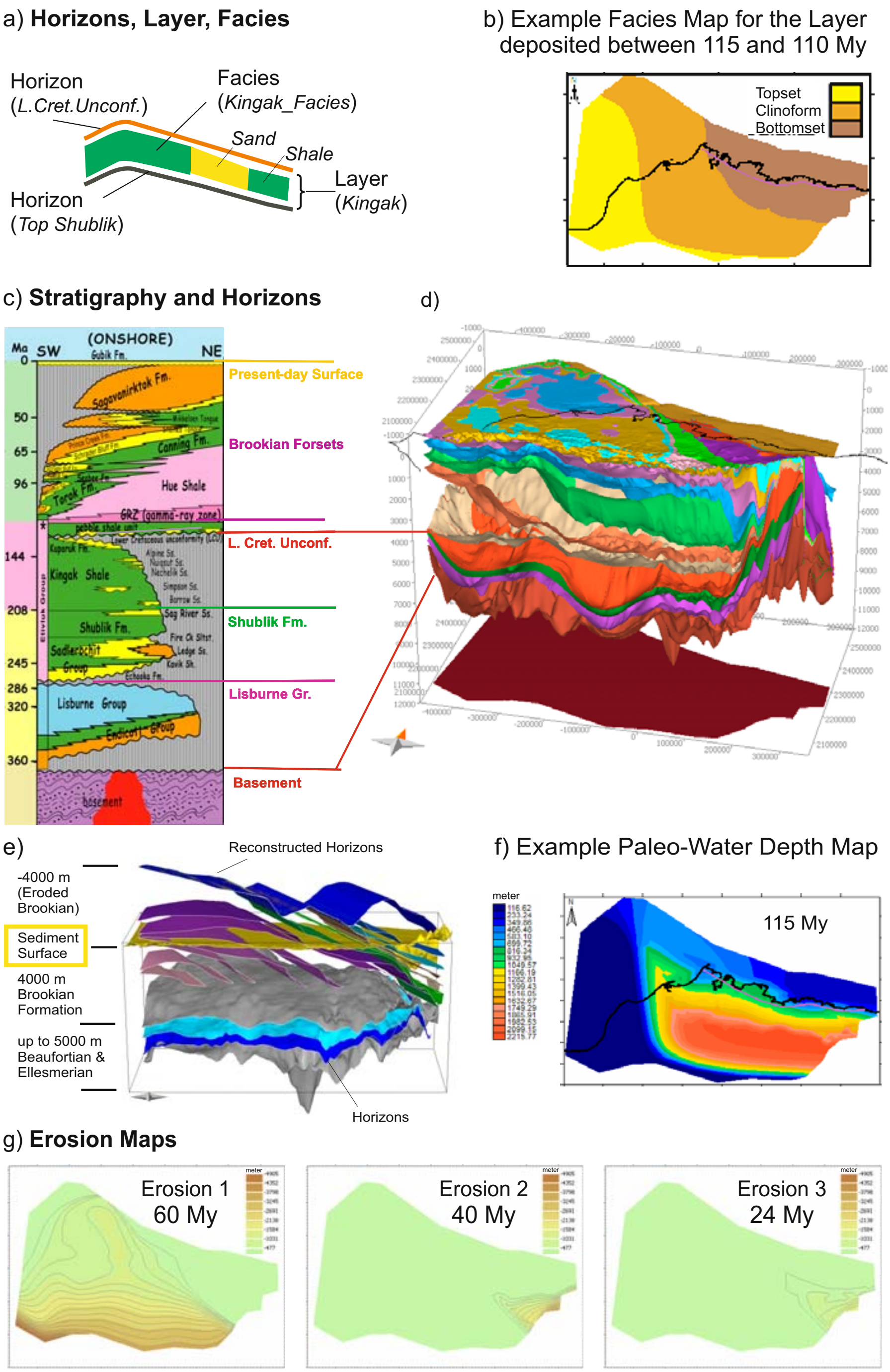

Fig. 1.3. Present day and paleo–geometry data: example from Alaska North Slope

A complete stack of horizon maps subdivides the space for volumetric property assignments. Parts of layers with similar sedimentation environments are called geological facies (Fig. 1.8). Facies are related to common property values of geological bodies. They are the main “material types” of the model. Layers can consist of several different facies and the same facies can appear in different layers. The distribution of facies is usually described with one facies map in each layer, based on well data information and sedimentological principles, e.g. clastic rocks are distributed corresponding to relationships between grain size and transport distances, particularly the distance from the coast (Fig. 1.3). In simple cases a layer can be characterized only by one unique facies type, whereas high resolution seismic facies maps allow the construction of very detailed facies maps (Fig. 1.10).

Fault planes are constructed from seismic interpretations, well data, and dips, which can also require a lot of effort. Depth horizons, facies maps, and fault planes constitute the present day model.

Age Assignment

The age assignment or stratigraphic table relates the present day horizons and layers with the geologic age of their deposition and erosion. In layer sequences without erosions, horizons represent all sedimentary particles, which are deposited during the same geological events (Fig. 1.3). If valid for the model, erosion and hiatus events also have to be included in the stratigraphic table. Erosion events require additional maps for the amounts of erosion and have to be combined with the corresponding water-depth for the description of the related uplift of the basin.

Stratigraphic diagrams with facies variations (Fig. 1.3) have to be simplified in order to get a relatively low number of model horizons in the range of $10-50$. Migrating patterns of facies through time generally require a Wheeler diagram instead of one single simplified age table. However, this feature is rather difficult to implement into a computer program.

Paleo-Geometry Data

The present day model can be built from measured data, such as seismic and well data. The paleo–model is mainly based on knowledge and principles from historical and regional geology, sedimentology and tectonics, which results in higher degrees of uncertainty. Water depth maps are derived from isostasy considerations of crustal stretching models together with assumptions on global sea level changes. They describe the burial and uplift of the basin. Water depth maps can also be derived from known distributions of sediment facies and vice versa (see e.g. the equivalence of the water–depth and facies map at 115 My in Fig. 1.3.b and f).

The construction of the erosion maps is usually more difficult. In the simplest case, one layer is partially eroded during one erosional event. The erosion thickness can be re–calculated by decompaction of the present day thickness and subtraction from an assumed relatively uniform depositional map. The

Age [My]	Horizon	Layer	Facies Maps	Erosion Maps	Paleo-Water Depth Maps
0	Present Day				PWD_0
		Brookian D	BrFac D		
24					PWD_24
		EROSION	*none*	**Erosion3**	
25	Top Oligocene				PWD_25
		Brookian C	BrFac C		
40					PWD_40
		EROSION	*none*	**Erosion2**	
41	Top Lutetian				PWD_41
		Brookian B	BrFac B		
60					PWD_60
		EROSION	*none*	**Erosion1**	
65	Top Upper Cretaceous				PWD_65
		Brookian A	BrFac A		
115	Top Lower Cretaceous				PWD_115
...	...	...	...		...
126	L.Cret.Unconf.				...
		Kingak	Kingak_Facies		
208	Top Shublik				...
		Shublik	Shublik_Facies		
260	Top Lisburne				
		Lisburne	Lisburne_Facies		
360	Top Basement				
		Basement	Basement_Facies		
400	Base Basement				

Fig. 1.4. Excerpt from the age assignment table of the Alaska North Slope model

sediment surface of the example model in Fig. 1.3.d acts as a unconformity and cuts many layers. A simple approach is to construct the missing erosion amount for each layer separately and to assume uniform erosion during the time period of erosion. This is illustrated in Fig. 1.3.e with the virtual horizons of the Brookian formation above the sediment surface. However, in the considered model it is further known that there were three main erosion periods and thus the corresponding erosion maps could be constructed (Fig. 1.3.g.). These maps together with the virtual Brookian horizons yield the erosion amounts for each of the layers in the three erosion events.

The above model description would have been sufficient, if the Brookian formation were eroded after complete deposition. In reality, compressional deformation in the Tertiary produced a fold–and–trust belt resulting in uplift and erosion and in a broad shift of the basin depocenters from WSW to ENE, which lead to mixed erosion and deposition events. A schematic description is illustrated in Fig. 1.5 which is finally realized in the age assignment table of Fig. 1.4. Note, that each erosion mentioned in the age assignment table consists of several layer specific maps with the erosion amounts related to the respective event. Unfortunately, such a complicated behavior is rather typical than exceptional. Input building tools often provide sophisticated map calculators with special features to make the construction of erosion maps easier. A preliminary simulation result of an ongoing Alaska North Slope study is shown in Fig. 1.6.

The occurrence of salt diapirs requires paleo-thickness maps for the main phases of salt doming. The reconstruction of the salt layers is usually based on geometrical principles, in the simplest case the present day thickness map

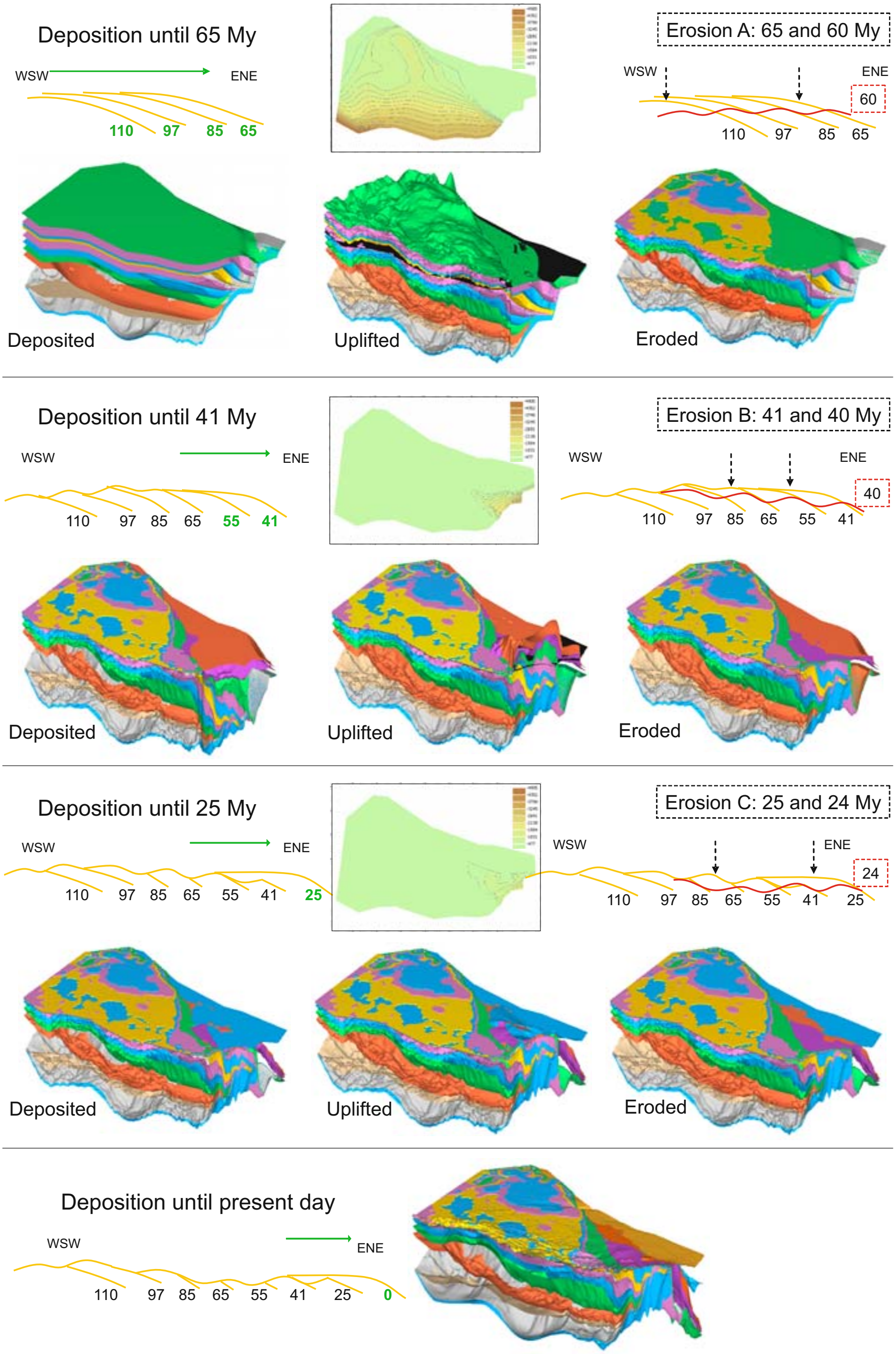

Fig. 1.5. Paleo–geometry data: example from the Alaska North Slope

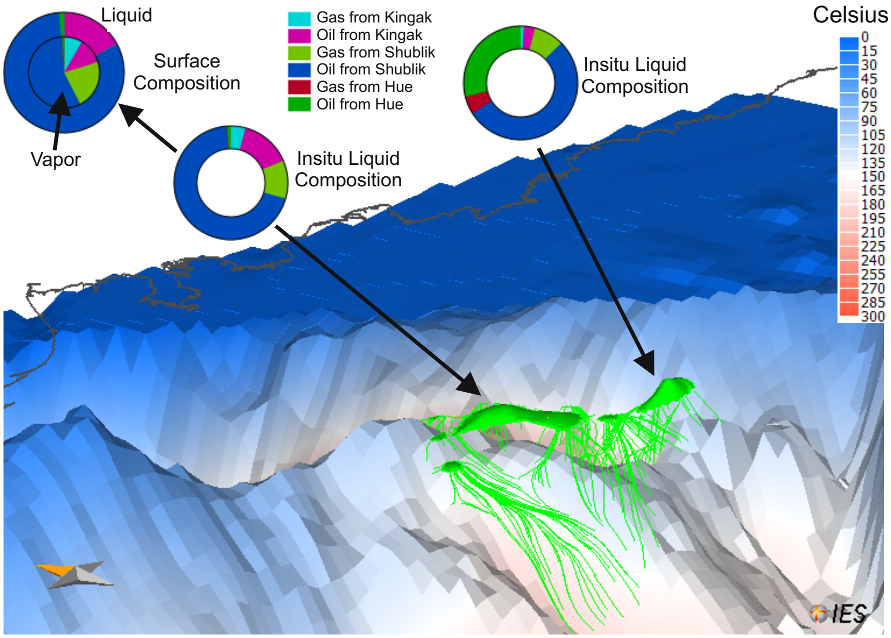

Fig. 1.6. Source rock tracking in Alaska North Slope. The two big visible accumulations are the Kuparuk (center) and Prudhoe Bay (right) fields

is linearly interpolated to an uniform deposition map. Corrections are made, if the resulting paleo-geometries show unrealistic kinks in the reconstructed base–salt maps. Salt layers can also be reconstructed based on calculated lithostatic pressures or total stresses at the salt boundaries because salt moves along the gradient of the lowest mechanical resistivity. The reconstructed salt thickness maps can be implemented in the input model by two methods: paleo–thicknesses for autochthonic salt layers and penetration maps for allochthonous salt bodies as illustrated in Fig. 1.7 for the Jurassic salt layer of the Northern Campos Model. Autochthonous salt maps through geologic times can be simply realized by adjusting the layer thickness in each gridpoint. The occurrence and timing of the salt windows is often very important for petroleum migration and pressure development as subsalt fluids and pressures are released afterwards.

The penetration of shallower sediments by salt and the formation of single allochthonous salt bodies is usually implemented with the replacement of the original sediment facies by the salt facies. Both methods have to be combined with adjustments of the other sediment thicknesses to maintain the mass balance. These correction maps can be added to the input data as paleo-thickness maps during the corresponding events.

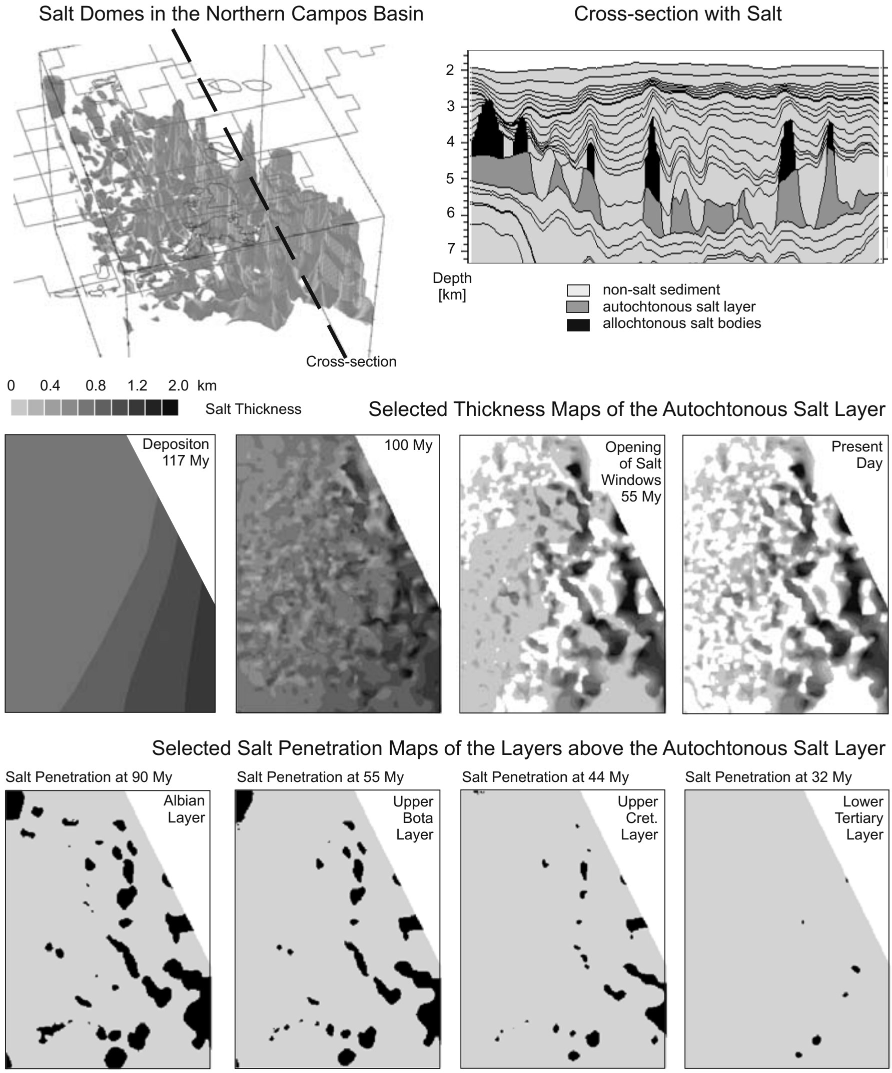

Fig. 1.7. Paleo–salt maps: example from the Northern Campos Basin in Brazil

The interplay of paleo-water depth, erosion, salt thickness, and other paleo-thickness maps finally determines the paleo-geometries and often requires some experience of the basin modeler to build geological reasonable scenarios.

Boundary Conditions

Boundary conditions need to be defined for the heat, pressure, and fluid flow analysis through the entire simulated geologic history. The usual boundary condition data for the heat flow analysis are temperature maps on the sediment surface or the sediment–water interface and basal heat flow maps for the respective events. The surface temperature maps are collected from general paleo–climate databases. The basal heat-flow maps can be estimated from crustal models and calibrated with thermal calibration parameters, which is explained in more detail in Chap. 3. Specific inner and upper igneous intrusion temperature maps should be added for magmatic intrusion and extrusion events, respectively.

The boundary conditions for the pore pressure and fluid flow analysis are often defined as ideal open (e.g. at sediment surface) and ideal closed (e.g. at base sediment). Exceptions are onshore basins or erosion events, which require the definition of groundwater maps to calculate the groundwater potential as the upper boundary condition for the pore pressure analysis. Herein, the sediment surface could be a good approximation.

It is a common method to determine the boundary values through geologic history as trend curves at single locations (gridpoints) first and calculate boundary value maps for the geological events by inter– and extrapolation afterwards.

Facies Properties

Facies are sediment bodies with common properties. The name facies is widely used in geoscience for all types of properties. Here, the facies is characterized by two sub–group facies types: the rock facies (or lithology) and the organic facies (or organofacies, Fig. 1.8).

A classification of lithologies is also shown in Fig. 1.8. It is used for the rock property tables in the appendix. The main rock properties are thermal conductivities, heat capacities, radiogenic heat production, permeabilities, compressibilities, and capillary entry pressures. Most of them depend on temperature and porosity. Functions for fracturing and cementation are also rock specific properties.

A classification of the organic facies is discussed in Chap. 4. The organic facies encompass all kinetic parameters for the generation and cracking of petroleum and the parameters to specify the quantity and quality of organic matter. The kinetic parameters are mainly Arrhenius–type activation energy and frequency data for primary and secondary cracking of hydrocarbon components. The total organic content (TOC) and the hydrogen index (HI) are usually defined by distribution maps. Furthermore, adsorption parameters are also related to the organic facies type. Fluid properties are either given directly for the different fluid phases or calculated from compositional information. Fluid phase properties are e.g. densities or viscosities. Typical fluid component properties are critical temperatures, pressures, and specific volumes.

Seismic

Seismic attribute cubes or maps can be used to refine the facies distribution maps in some layers, e.g. the ratio of shear to compressional velocity is correlated to the average grain size of clastic rock. The conversion of seismic

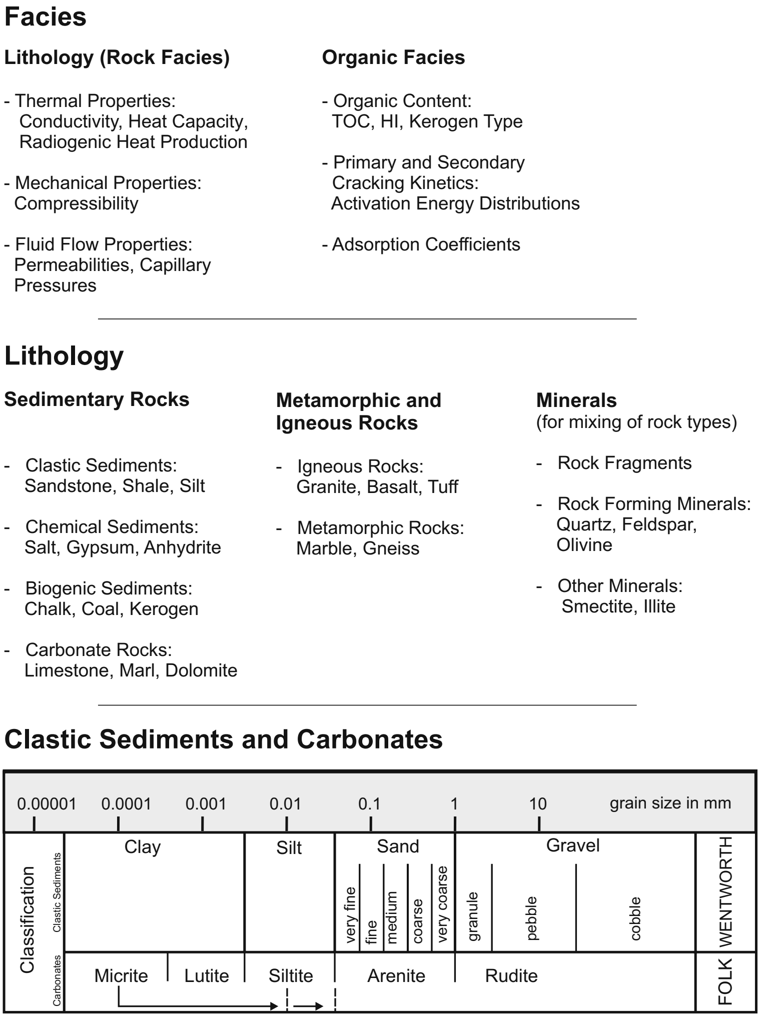

Fig. 1.8. Classification of facies, lithologies with the most important examples and terminology of clastic sediments and carbonates according to grain sizes. The picture is from Bahlburg and Breitkreuz (2004)

attributes to a "lithocube" requires a lot of effort and is only available in a few projects. Seismic facies cubes are usually available for the reservoir layers. In Fig. 1.9 and 1.10 two example cases from Australia and the North Sea are shown. Seismic facies cubes and maps are used, respectively. Seismic cubes can be given in two–way–time or depth. They require reference horizons to map the corresponding cells from the seismic to the depth model. The resulting facies distribution can be even finer than the major model grid. The