1

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.

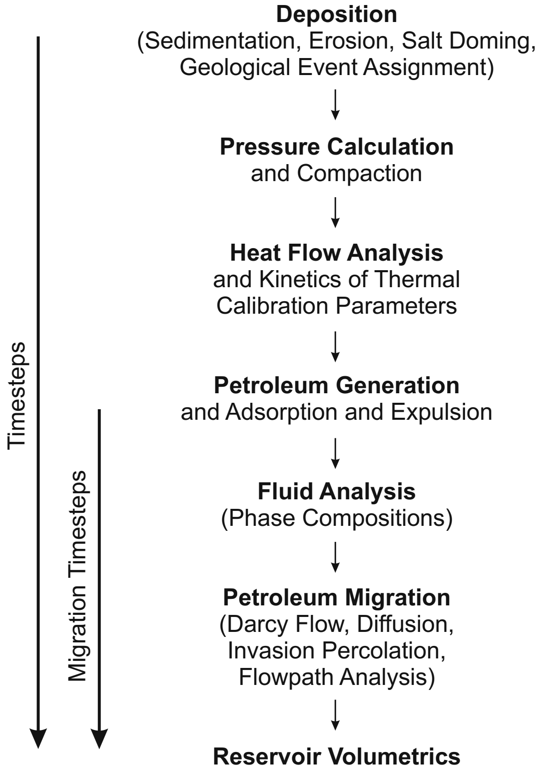

Fig. 1.1. Major geological processes in basin modeling

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 $\mathbf{v}_w$	$\mathbf{v}_w = -\frac{\mathbf{k}}{\nu} \cdot \operatorname{grad}(p - \rho g z)$	Permeability $\mathbf{k}$ and viscosity ν
Fluid potential u_p	Fluid flow $\mathbf{v}_p$	$\mathbf{v}_p = -\frac{\mathbf{k} k_{rp}}{\nu_p} \cdot \operatorname{grad} u_p$	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.

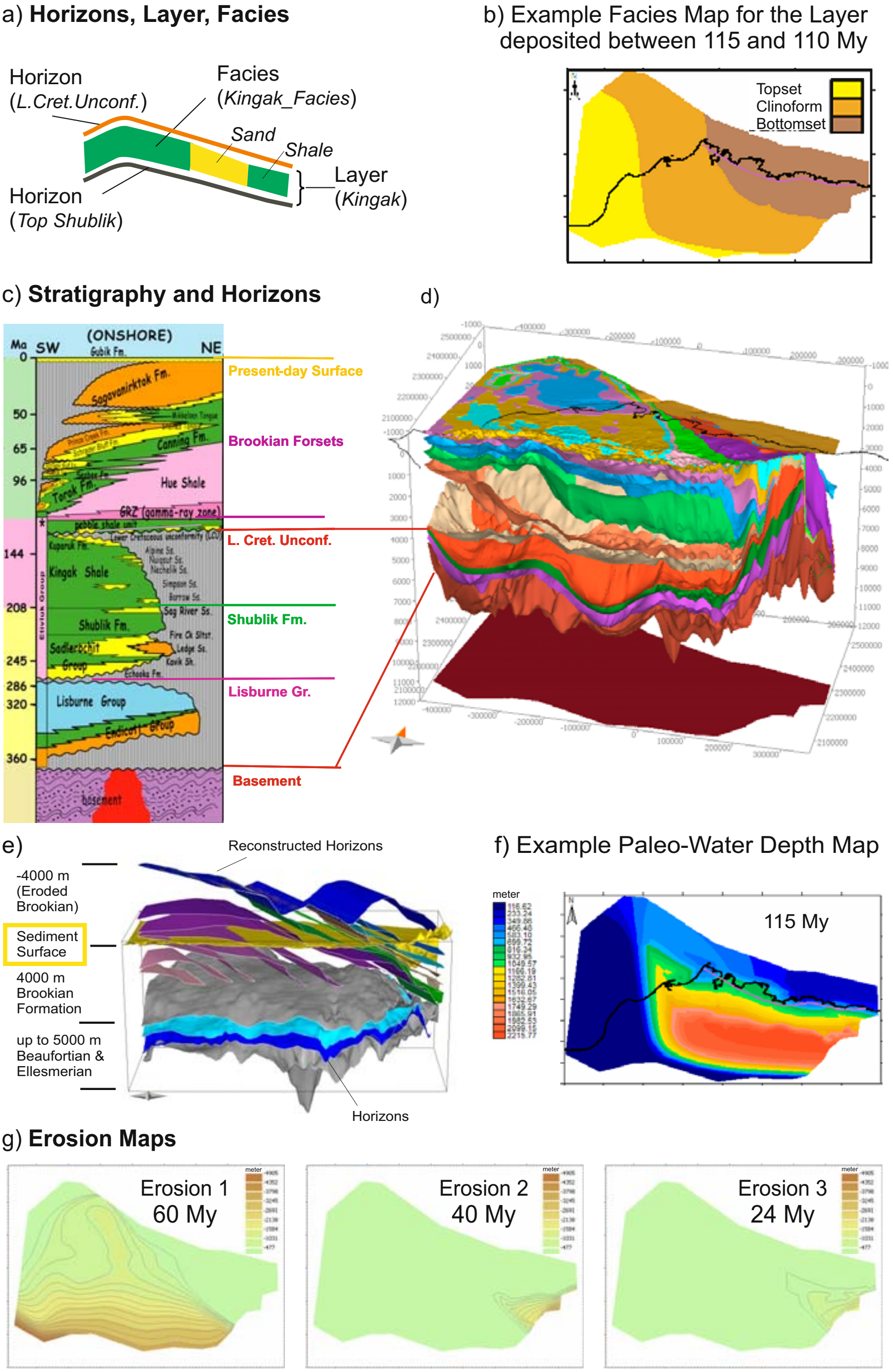

Fig. 1.3. Present day and paleo–geometry data: example from Alaska North Slope

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

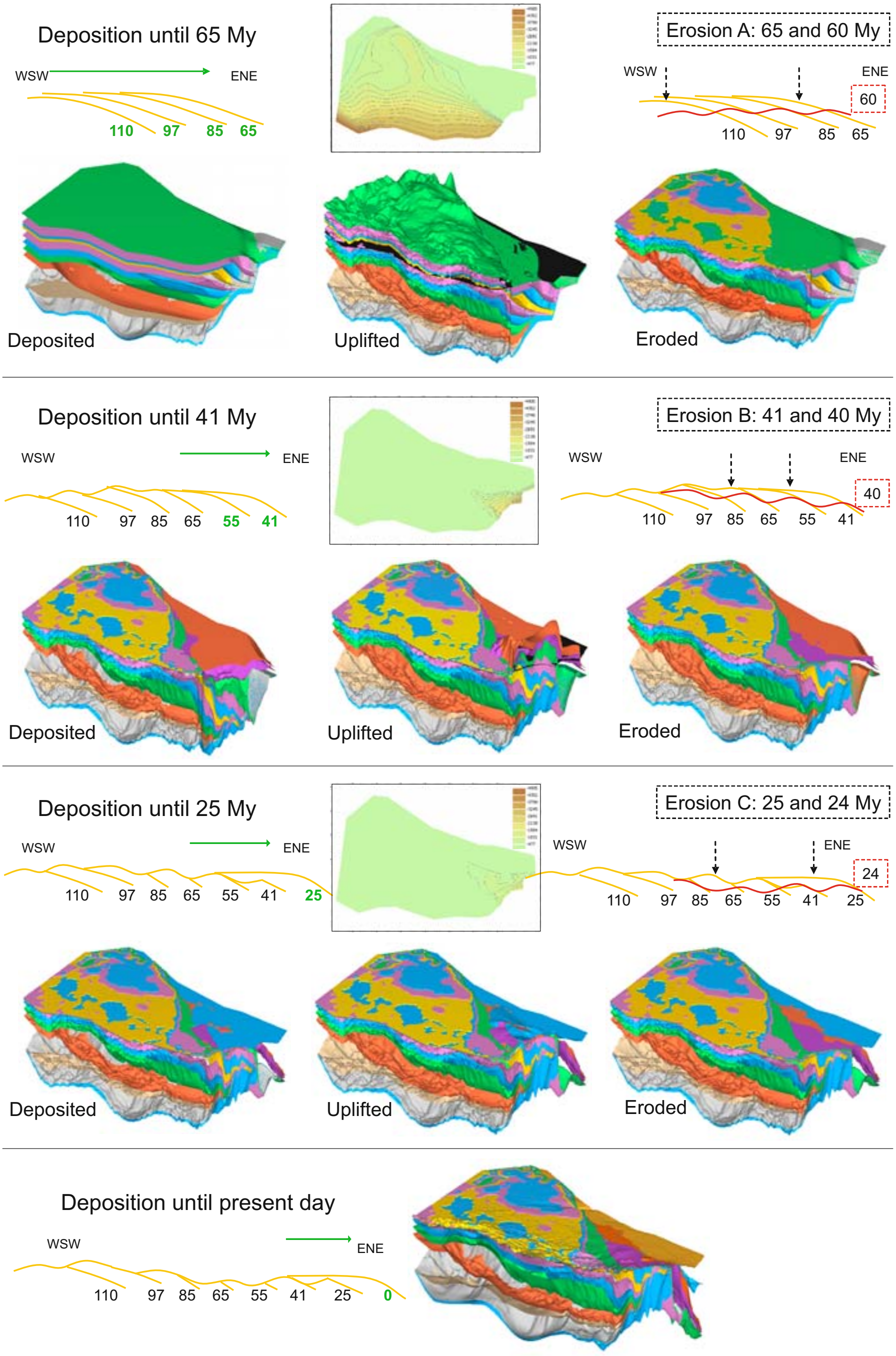

Fig. 1.5. Paleo–geometry data: example from the Alaska North Slope

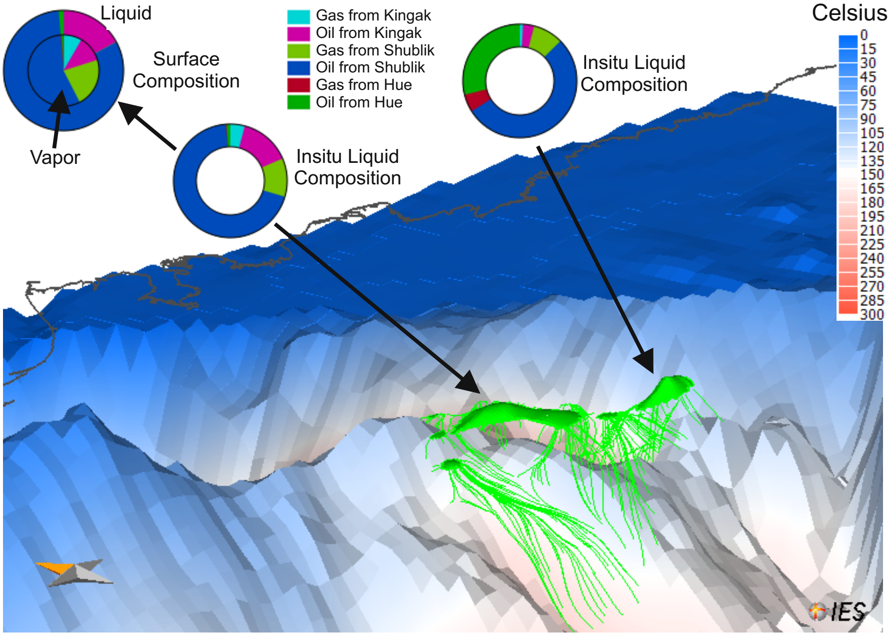

Fig. 1.6. Source rock tracking in Alaska North Slope. The two big visible accumulations are the Kuparuk (center) and Prudhoe Bay (right) fields

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.

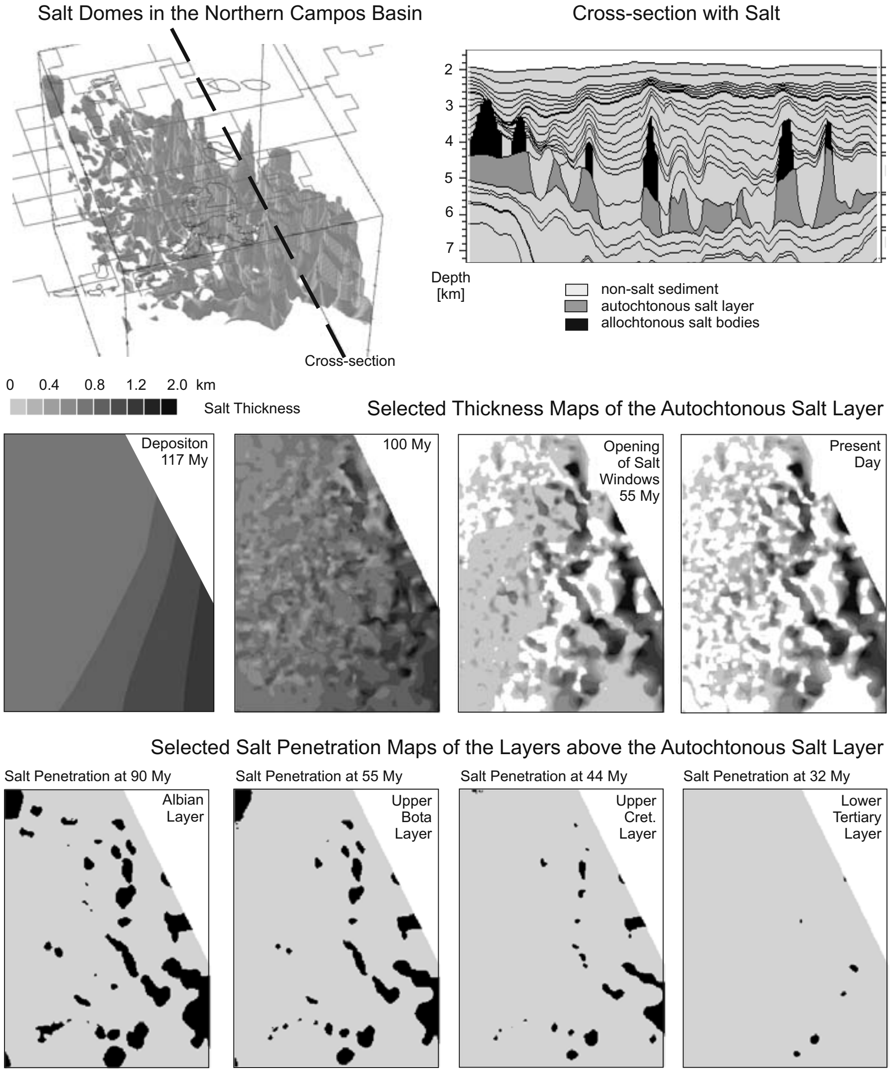

Fig. 1.7. Paleo–salt maps: example from the Northern Campos Basin in Brazil

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

Facies

Lithology (Rock Facies)

- Thermal Properties:
  Conductivity, Heat Capacity, Radiogenic Heat Production
- Mechanical Properties:
  Compressibility
- Fluid Flow Properties:
  Permeabilities, Capillary Pressures

Organic Facies

- Organic Content:
  TOC, HI, Kerogen Type
- Primary and Secondary Cracking Kinetics:
  Activation Energy Distributions
- Adsorption Coefficients

Lithology

Sedimentary Rocks

- Clastic Sediments:
  Sandstone, Shale, Silt
- Chemical Sediments:
  Salt, Gypsum, Anhydrite
- Biogenic Sediments:
  Chalk, Coal, Kerogen
- Carbonate Rocks:
  Limestone, Marl, Dolomite

Metamorphic and Igneous Rocks

- Igneous Rocks:
  Granite, Basalt, Tuff
- Metamorphic Rocks:
  Marble, Gneiss

Minerals
(for mixing of rock types)

- Rock Fragments
- Rock Forming Minerals:
  Quartz, Feldspar, Olivine
- Other Minerals:
  Smectite, Illite

Clastic Sediments and Carbonates

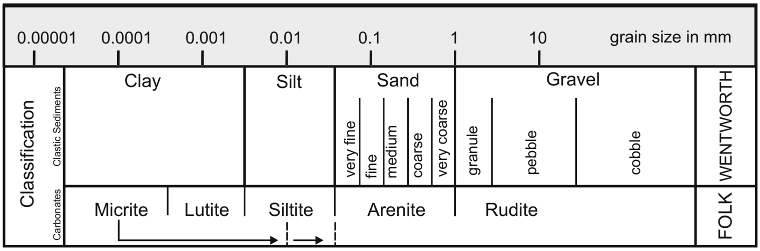

Fig. 1.8. Classification of facies, lithologies with the most important examples and terminology of clastic sediments and carbonates according to grain sizes. The picture is from Bahlburg and Breitkreuz (2004)

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 invasion percolation method, which is used for modeling of migration, works on a sub–gridding of the cells and takes high resolution features into account (Chap. 6). Capillary entry pressures from the finer scale seismic facies control migration and accumulation.

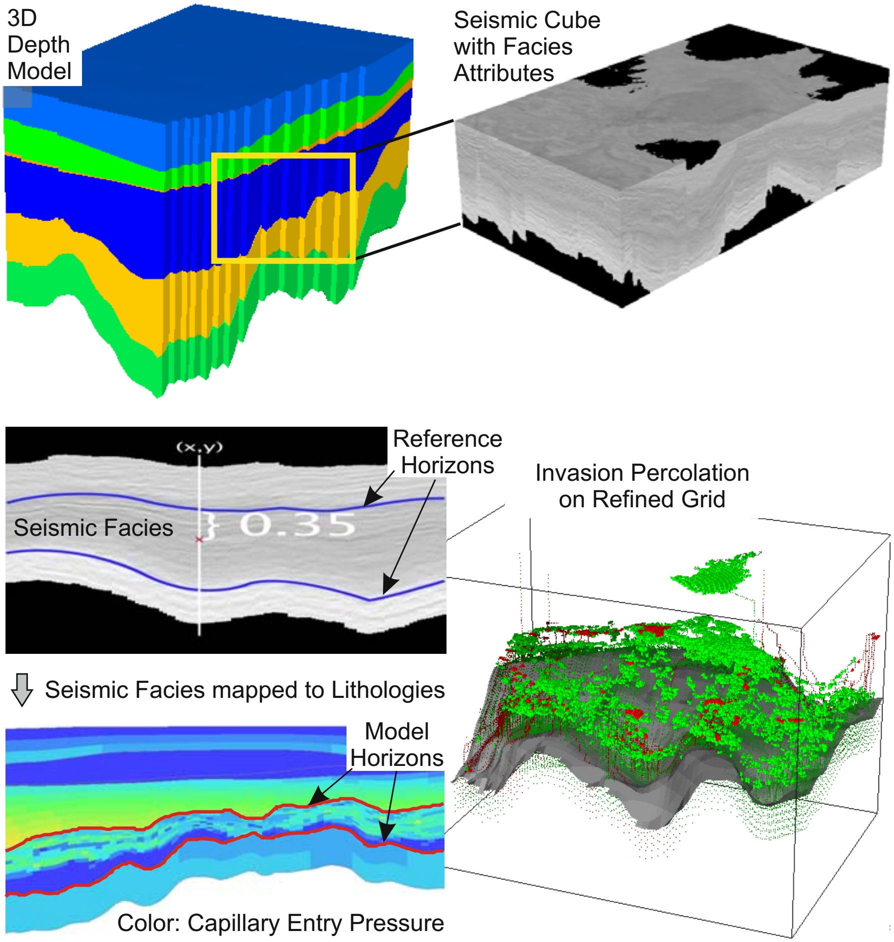

Fig. 1.9. Seismic cube with facies attributes and migration with invasion percolation. The attributes are mapped via reference and model horizons to the 3D model. For example, a point which lies at 35 % vertical distance between two reference horizons is here assumed to lie on the same relative position between the corresponding model horizons

The North Sea petroleum migration example (Fig. 1.10) is mainly restricted to two layers only: the upper Jurassic layer, and the overlaying chalk layer. The Jurassic layer contains high organic content shale and sandstone. It

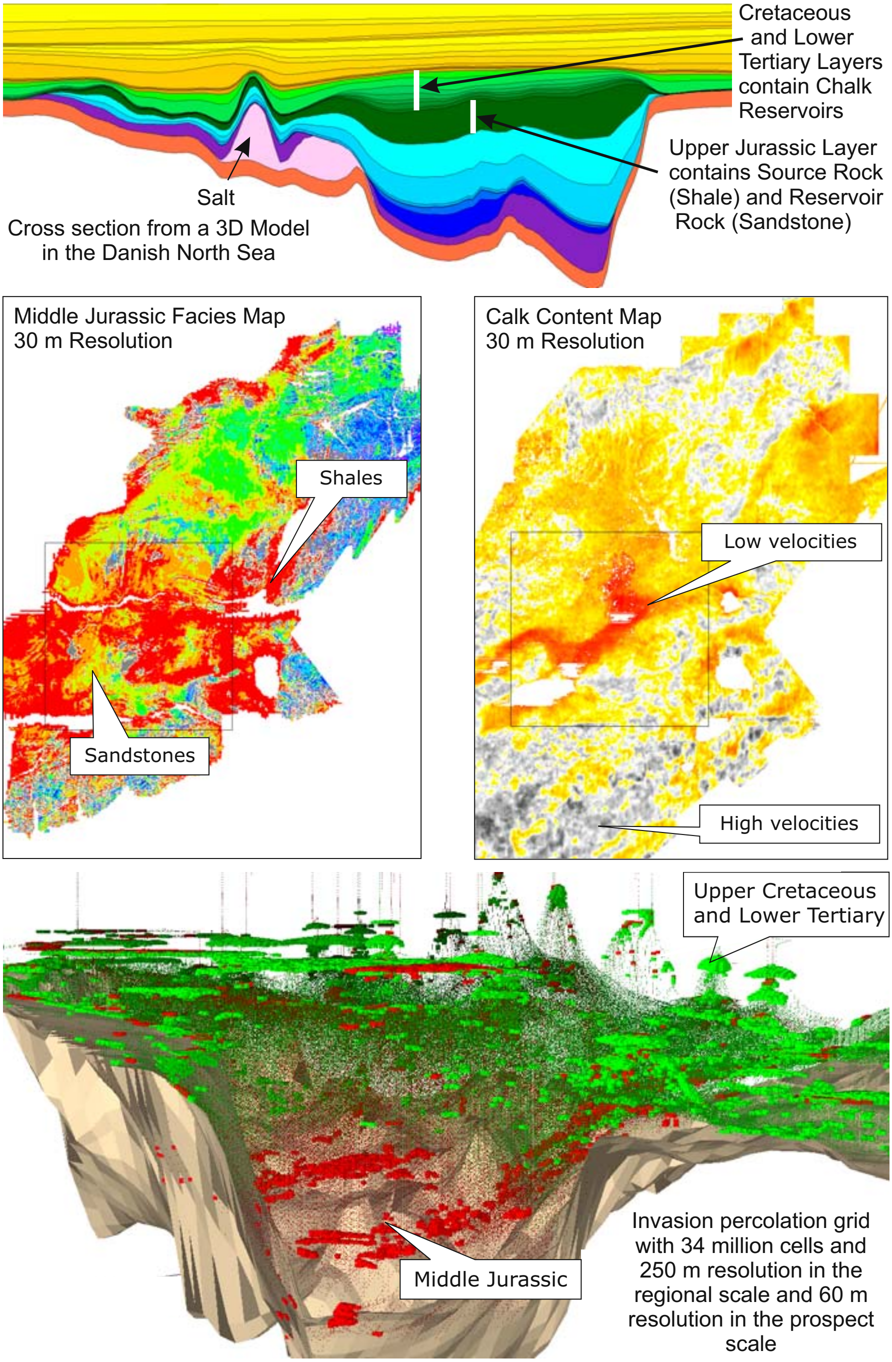

Fig. 1.10. High resolution maps and migration modeling with invasion percolation. The figures are courtesy of MAERSK

is both, a source and a reservoir layer. The chalk layer also contains petroleum accumulations and it is sealed by a dense overlaying shale. The two seismic attribute maps are applied to the layers without any further subdivision in vertical directions. In this case, the invasion percolation method is especially suitable, as high resolution is important and the migration distances are short.

Discretization of a Model

A continuum approach is commonly applied for the general description of heat and fluid flow processes on a macroscopic scale. Practical solutions can, on the other hand, only be obtained for discretized models. A mesher generates grids with the cells as the smallest volumetric units of the geological model. The basin or region of interest is assumed to be covered continuously with cells. Every physical or geological quantity such as temperature, pressure, saturation, concentration, permeability, thermal conductivity, etc. is well defined in the cell as a single, effective or average value. Furthermore, the value can vary continuously from cell to cell at least within parts of the structure. Each cell is used as a finite element or finite volume within the mathematical solvers.

The approach requires that the size of the cell must be small compared to the system being modeled (basin scale) but, at the same time, large compared to the pore scale and grain size. Typical scale sizes are

Molecular Scale: $10^{-9} \dots 10^{-8}\,\mathrm{m}$
Pore Scale: $10^{-6} \dots 10^{-3}\,\mathrm{m}$
Bulk Continuum: $10^{-3} \dots 10^{-2}\,\mathrm{m}$
Cells of the Grid: $10^{0} \dots 10^{2}\,\mathrm{m}$
Basin Scale: $10^{3} \dots 10^{5}\,\mathrm{m}$

with cells which are much larger than the pore scale and grain sizes and much smaller than the basin scale.[1]

However, modern simulation programs might contain different grid scales and even different basin scales for the modeling of different geological processes. Such multigrids are typically created with sampled and refined representations of a master grid. Optimal methods can then be applied for each geological process. For example, heat flow is often modeled on the full basin scale with grid cells seldom smaller than 100 m, whereas petroleum systems modeling is sometimes restricted to smaller areas of source rock expulsion and active migration pathways with corresponding grid cells, which can become very small. However, sophisticated up- and downscaling functions (e.g. for fractal saturation patterns) may be required.

Many quantities can be defined as gridded maps at certain events. Alternatively, geological time dependent trend functions are often specified at

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[1] In finite element simulators, a continuous crossover within a cell is modeled and the bulk continuum scale, rather than the cell size of the grid, must be compared with the basin scale. Finite elements therefore often show an implicitly higher resolution than other cell types.

individual well locations. Maps are then generated for each event by spatial interpolation over the whole model area. In both cases maps are the central objects for the creation of a basin model.

Size of a Model

A primary target of basin modeling is the assessment of exploration risk by calculation of generated and accumulated petroleum volumes for different geological migration scenarios. Herein, basin to reservoir scale models are used from a total length of hundreds of kilometers down to only a few kilometers (Fig. 1.11). Another study type concerns resource assessments, which cover even more extensive geographical areas such as entire countries (Fig. 1.11). The total amount of oil and gas resources in several layers is estimated. This task often encompasses source rock maturity studies including volumetrics for migration losses with simplified reservoir distributions. Governmental geological surveys and academic institutes often contribute to such studies.

Typical model dimensions and grid data are shown in Fig. 1.11. In practice, there are in general two requirements, a minimum model resolution to approximate the geological structures of interest and a simulation run time of less than 12 hours. This is a “rule of thumb” of the authors: a simulation must to be able to run in one night.

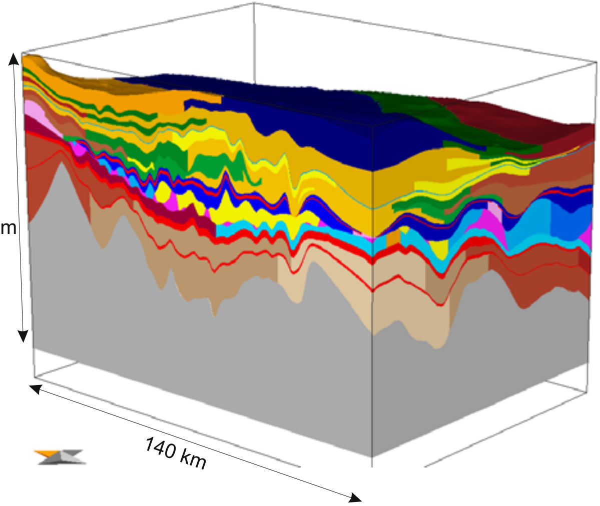
Computer performance has significantly increased since the introduction of parallelized simulations on computer clusters. The average number of cells for a complete simulation is $1-2$ million cells which corresponds to $200-300$ gridpoints in the horizontal directions. Heat, pressure, and Darcy flow computing times depend almost exponentially on the number of cells. Doubling the number of gridpoints in one direction often increases the computing effort by one order of magnitude. That is why big improvements in computer performance and numerical methods often have only a small effect on the grid resolution. However, computing time is very difficult to estimate as some important controlling parameters, such as the number of hydrocarbon containing cells, average and peak fluid flow rates or the number of migration time steps for good convergence, are not known prior to the special conditions of each simulation.

1.4 Petroleum Systems Modeling

A “Petroleum System” is a geologic system that encompasses the hydrocarbon source rocks and all related oil and gas, and which includes all of the geologic elements and processes that are essential if a hydrocarbon accumulation is to exist (Magoon and Dow, 1994).

A petroleum systems model is a digital data model of a petroleum system in which the interrelated processes and their results can be simulated

Exploration Risk Assessments - Northern Campos Basin (Brasil)



Maps: 20..50

Grids: 100..500 x 100..500

Cells: 0.1 .. 4 Million

Cell Size: 100..2000 m

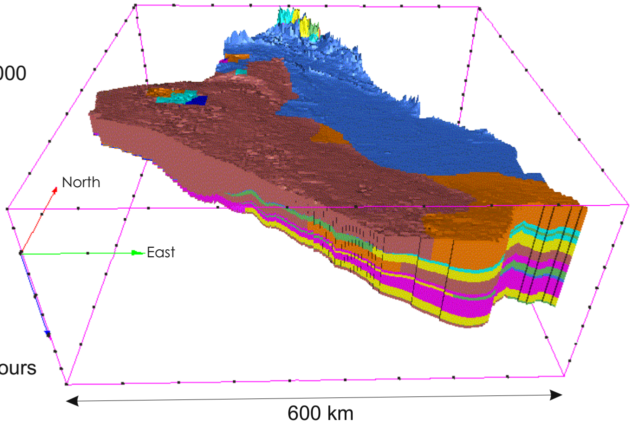
Timesteps: 2000..20000

Processors: 1..10 (..20 for Risk Runs)

Analysis: Petroleum System

Computing Time: 1..12 hours

Hydrocarbon Resource Assessment (Iraq)



Maps: 20..50

Grids: 500..1000 x 500..1000

Cells: 1 .. 10 Million

Cell Size: 2 km ..50 km

Timesteps: 200..2000

Processors: 4..10

Analysis: Source Rock

Computing Time: 10..30 hours

Fig. 1.11. Studies on prospect and regional scales. The figure from Iraq is courtesy of the U.S. Geological Survey and described in Pitman et al. (2003)

in order to understand and predict them. It is a preferably 3D representation of geological data in an area of interest, which can range from a single charge or drainage area to an entire basin. A petroleum systems model is dynamic which means that petroleum systems modeling provides a complete and unique record of the generation, migration, accumulation and loss of oil and gas in a petroleum system through geologic time.

Petroleum systems modeling includes basic assessments such as:

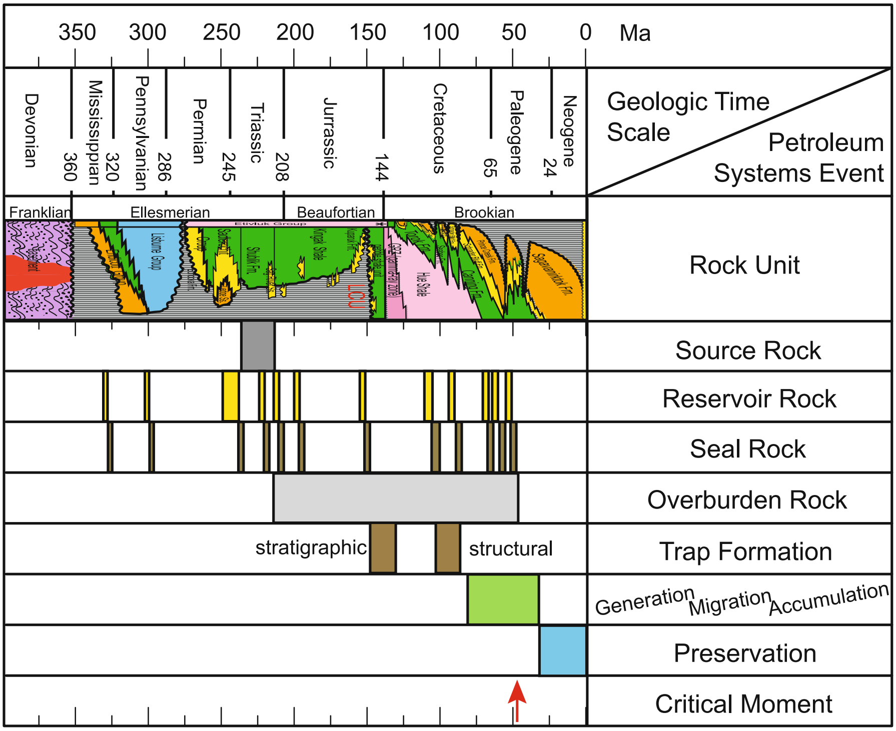


Fig. 1.12. Simplified petroleum system chart of Alaska North Slope after Magoon et al. (2003)

Have hydrocarbons been generated? This includes a full range of services from initial charge risking in frontier areas to regional resource assessments of yet–to–find hydrocarbons.

Where were hydrocarbons generated? If hydrocarbons were generated, their locations can be defined quite accurately so that their possible relationships to prospects can be risked.

When were hydrocarbons generated? There are many clear examples of where basins, plays, and prospects have failed due to timing problems. For example, when oil and gas was generated early and the structures were created much later.

Could hydrocarbons have migrated to my prospect? Modeling of the dynamic process of generation, expulsion, and migration makes it possible to determine if the oil and gas charge could reach the trap.

What are the properties of the hydrocarbons? Modeling of the phase behavior of the hydrocarbons during migration, accumulation and loss makes it possible to determine oil vs. gas probabilities and even predict properties such as API gravities and GORs.

Petroleum systems modeling can be interpreted as a sub-group of basin models, which model the full hydrocarbon lifecycle. It covers the most sophisticated targets of basin modeling.

Each source rock develops its own petroleum system. The petroleum system elements are facies, which contained, transported or sealed the generated petroleum from one source rock. These facies were named according to their function as source rock, carrier rock or seal. All the distributed petroleum of one petroleum system is more or less connected with rest saturation drops, migration stringers and accumulation bodies (Fig. 1.10) and is usually mixed with other petroleum systems from the same basin. The petroleum system chart shows the timing of the petroleum systems elements and allows a first assessment of the process chain (Fig. 1.12).

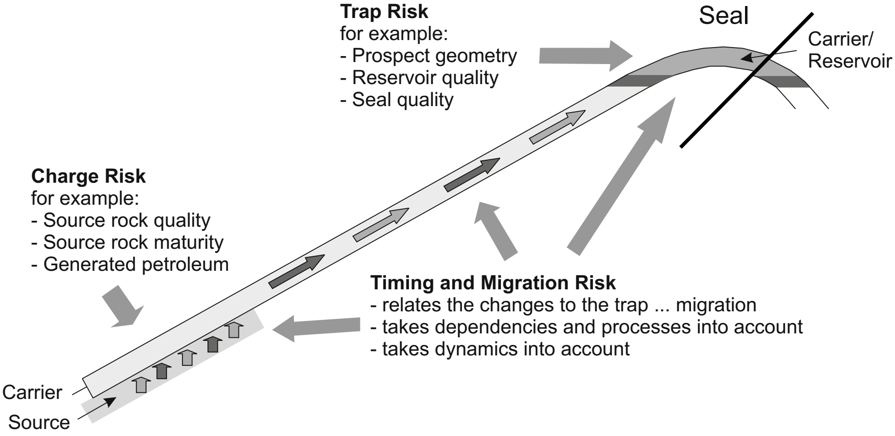


Fig. 1.13. Risk factors of petroleum systems modeling

A primary target of petroleum systems modeling are hydrocarbon exploration risk factors (Figs. 1.13, 1.14). They are the hydrocarbon charge, the reservoir quality, the trap capabilities and the timing relationship between the charge, reservoir, and seal (Fig. 1.13). Exploration risk commissions often evaluate the risk related to charge, reservoir, and seal, separately and subdivided into several factors (Fig. 1.14). Obviously, most of these risk factors can be assessed from a well designed basin model with special emphasis to the charge factors. Probability analysis methods (Chap. 7) allow the total risk to be quantified as a result of special uncertainties of the single risk factors and also take into account the timing relationships. Thus, basin modeling combined with probability analysis can be used as a decision support system for exploration risk assessment.

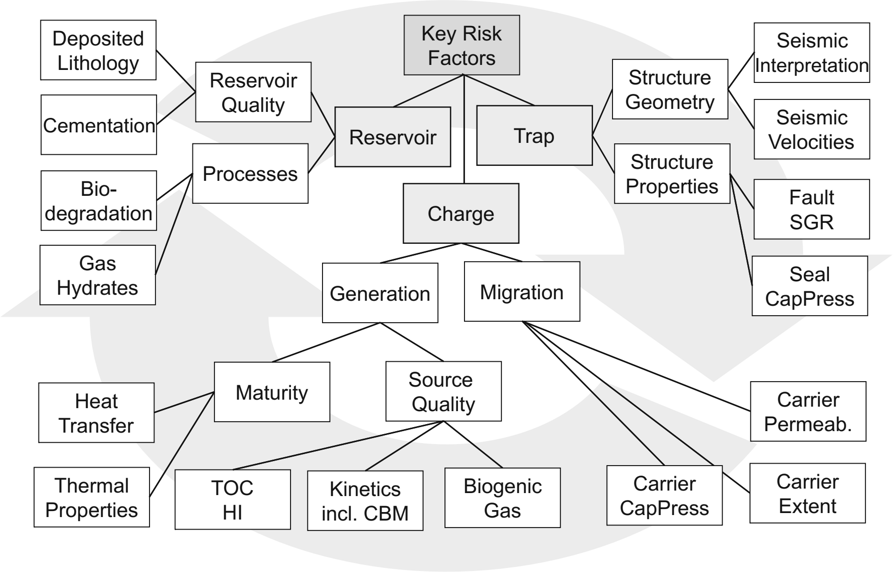


Fig. 1.14. Petroleum Systems Modeling as a Decision Support System

1.5 Modeling Workflows

The employment of some geological processes is optional and sometimes modeling of pressure or migration is not needed. It also makes sense to completely decouple pressure, temperature, and hydrocarbon fluid flow modeling from each other especially for pressure and temperature calibrations or if several migration scenarios should be tested. The following schemes for source rock analysis, reservoir volumetrics, and migration modeling demonstrate some common workflows (Fig. 1.15).

Source Rock Maturation Study

This type of study is performed when knowledge about the basin is sparse or when project deadlines are near. Large uncertainties in the data may not allow a sophisticated modeling. Only basic facts are investigated and emphasis is put on small simulation times.

In the initial step a model is calibrated for pressure and then again for temperature.[2] Both calibrations are performed fully decoupled. Feedback of temperature effects on compaction are not taken into account. This enhances the performance of the procedure drastically. Possible errors are neglected.

After the calibration, generated hydrocarbon masses give a first idea about source rock maturity, peak expulsion times and maximum reservoir fillings.

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[2] It is important to perform the pressure calibration before the heat flow analysis since pressure formation influences the paleo–geometry which can have a significant effect on temperature history.

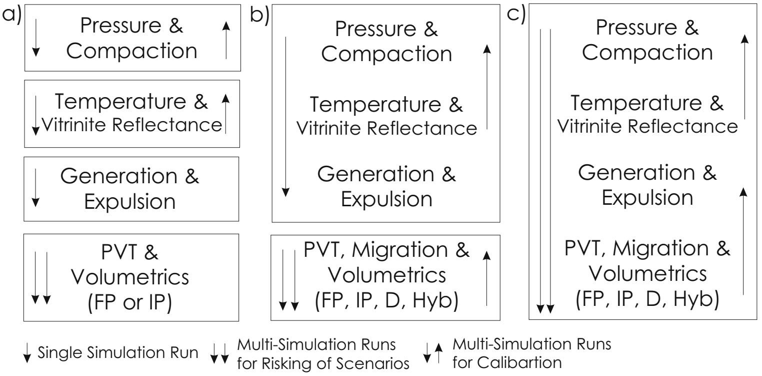

Fig. 1.15. Modeling Workflows for (a) Source Rock Maturation Study. (b) Decoupled Migration Study. (c) Petroleum Migration Study. (FP..Flowpath Modeling, IP..Invasion Percolation, D..Darcy Flow Modeling, Hyb..Hybrid Flow Modeling)

Drainage areas of interest in the reservoir are mapped to the source rocks with some simple procedures and the corresponding expulsion amounts are collected for the volumetrics. Flowpath modeling and invasion percolation techniques can be used additionally in a more advanced manner to consider losses, spill and seal break through amounts.

Multi–simulation runs are often performed for calibration and inversion. Statistical methods can be used to improve the calibration workflow. Histograms with generated amounts are often evaluated as functions of uncertain parameters, such as basal heat flow or SWI temperatures. However, this type of modeling is too crude for risking of individual accumulations.

Decoupled Migration Study

A decoupled migration study is typically performed when multiple migration scenarios are studied. It is often not reasonable to recalculate compaction and temperature for each migration scenario anew because feedback effects between migration and compaction or temperature are usually very small. On the other hand, a lot of simulation time is saved when the pressure and temperature field is not recalculated for each simulation run.

Migration and accumulation are performed on the most sophisticated level. They are considered in more detail than in a source rock maturation study. The selection of the migration model depends on the type of the geological migration process, the model input, the available computer soft- and hardware and the output preferences of the user. Very often different migration methods are tested for their performance in a given basin under certain geological conditions. Darcy flow with time control is often applied, especially as a part of the hybrid migration method. For example, a petroleum system very often consists of several sources. The interaction of different reservoir layers can play an important role. Especially the charging of traps can be studied with the hybrid migration method. A large part of this book deals with explanations and comparisons of the different migration modeling methods.

Multi–simulation runs are performed to explore the range of calculated reservoir fillings dependent on unknown input parameters of the petroleum system. Statistical models are often applied to quantify the risk assessment procedure (Chap. 7).

Coupled Migration Study

The decoupled mode ignores the influences of the petroleum system on temperature and pressure, such as gas generation pressure or oil and gas influences on thermal conductivities. Coupled scenarios ensure modeling of the full interaction. Of course, high resolution 3D models need a lot of computer power for such fully integrated runs, especially when multi–simulation runs are needed for calibration and risk assessment. The calibration of the petroleum system is also part of the procedure when information about known accumulations is available. It cannot be done automatically since there are too many uncertain input parameters which affect the resulting accumulation pattern.

Workflows for modeling geological processes are numerous and most people have their own preferred data and workflows to achieve the desired results. There is no doubt that many of the controlling geological factors involved in these processes are not very well known and difficult to quantify, and that this limits the numerical accuracy of the models. For example, it is still unclear how short–term thermal events ("heat spikes") influence the kinetics of petroleum formation, or how significant errors in the heat flow history that result from insufficient knowledge of the intensity and time of erosional phases can be avoided. Additional restrictions are our limited knowledge of factors affecting carbonate diagenesis (early or late diagenetic cementation?), and subsequent inaccurate estimates of thermal conductivities at the respective diagenetic stages. This list can surely be extended. In many cases, it can be assumed that uncertainties resulting from missing knowledge about uncertain processes are often larger than small errors due to a missing feedback effect. More conceptual models with less coupled processes can be understood, calibrated, and studied more easily. For example, due to higher simulation performance more uncertain parameters can be varied to assess their influence on the modeling results.

1.6 Structural Restoration

Structural restoration deals with the determination of the shape of geological structures at paleo times. Overthrusting and faulting are the main topics. It is often performed with a backstripping approach which is mainly based on the mass and volume balances of rock material.

Structural restoration is tightly linked to basin modeling as the shapes of layers and faults are often used as inputs in basin modeling. Optimization procedures for geometry calculations can then be omitted. However, multiple simulation runs cannot be avoided if porosity is to be calibrated. Fully restored geometries of basins at certain events are needed and extensive restorations have to be performed (Chap. 2).

Structural modeling, geomechanics, and tectonics incorporate the modeling of stresses and strains. They are needed when fault properties, fracturing, and lateral effects on compaction are of interest.

1.7 Comparison with Reservoir Modeling

A role, similar to that of basin modeling in exploration, has traditionally been played in production by reservoir modeling (Aziz and Settari, 1979). There are many fundamental similarities between reservoir modeling and basin modeling, as both technologies are used to model transport processes for hydrocarbon fluid flow in geologic models in order to provide an improved understanding, so that better predictions of possible results can be made.

The scaling of basin and petroleum systems models is however completely different than that of reservoir models, as dynamic geologic processes are considered in basin modeling. Sedimentary basins evolve through geologic time with significant changes in their geometries due to burial subsidence and compaction, uplift, and erosion, and structural complexities. Additionally, the size of sedimentary basins is also orders of magnitude larger than typical field sizes. For example, mega-regional models cover areas the size of the Gulf of Mexico and include the entire sedimentary sequence up to depths of 10 km and more. As a result, pressure and temperature conditions in sedimentary basins vary over a much wider range.

Besides this there are some other fundamental differences which are less important from a technical viewpoint. For example, reservoir modeling deals with forecasts of future production.[3] The Influence of humans on the results, e.g. due to the injection of steam, play a central role. In contrast basin modeling is performed for geological times only. Human influences on the basin are obviously of no interest. Likewise an optimization routine, which is not found in reservoir modeling, is necessary for calibration of the present day geometry. Despite all these differences, basin modeling has benefited greatly from reservoir modeling. For example, fluid analysis was first applied in reservoir modeling and has now evolved to become a sophisticated addition to basin modeling.

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[3] History matching is similar to calibration in basin modeling. It is performed to improve the quality of future predictions.

1.8 Outlook

Future trends in basin modeling will involve the refinement of the implementation of all the above listed geological processes. As already mentioned there are, for example, developments for the integration of stresses and strains into simulators. This example is an enhancement of compaction and pore pressure prediction.

Besides this there are other developments which try to incorporate seismic information more directly into basin models. For example, invasion percolation models have a higher resolution than other processes in basin models. The resolution approaches almost the resolution of seismic data. A direct incorporation of seismic data is therefore desired.

Seismic data can also be used in general for facies and lithology assignment. However, appropriate attribute analyses and upscaling laws must be developed.

Summary: Basin modeling is dynamic forward modeling of geological processes in sedimentary basins over geological time spans. It incorporates deposition, pore pressure calculation and compaction, heat flow analysis and temperature determination, the kinetics of calibration parameters such as vitrinite reflectance or biomarkers, modeling of hydrocarbon generation, adsorption and expulsion processes, fluid analysis, and finally migration.

Transport processes for water (pore pressure and compaction), heat (temperature calculation), and petroleum (migration and diffusion) can be formulated in terms of flow equations with appropriate conservation equations for mass or energy which finally yield diffusion type differential equations.

A sedimentary basin is a sequence of geological layers. Each layer was deposited in a given stratigraphical event and is subdivided into regions of similar facies. A facies type specifies the lithological rock type and the organic facies. The lithology includes quantities such as permeability, compaction parameters, heat capacities, thermal conductivities and so on. The organic facies contain the total organic carbon content (TOC), the hydrogen index (HI) and the specification of the kinetic for petroleum generation. Boundary conditions must also be defined. Basal heat flow can be determined from crustal models for basin evolution.

Migration is the most sophisticated process in modeling. Due to its uncertain nature and extensive computing requirements different modeling approaches exist. Hybrid simulators combine the advantages of all approaches.

Additionally, a basin model contains special submodels concerning faults and fault properties, cementation, thermal calibration parameters, salt movement, intrusions, fluid phase properties, secondary cracking, and so on.

Basin models typically cover areas about 10 x 10 km up to 1000 x 1000 km and to a depth of 10 km. They are gridded into volume elements with up to 500 gridpoints in the lateral directions and up to 50 layers. Each volume element contains a constant facies in a bulk continuum approximation. Appropriate upscaling of physical properties from core to grid size might be necessary.

In practice, different workflows for risk evaluation and calibration exist. Dependent on the quality of the data, the geological processes are modeled decoupled, partially coupled or fully coupled. Source rock maturation studies are typically decoupled and petroleum migration studies are fully coupled. In between, decoupled migration studies are performed for risking, when, for example, the migration pathways are not known and different migration scenarios are tested.

Structural restoration yields valuable information about overthrusted layers and faulted geometries. It is an important step for modeling many of the world's basins.

Basin modeling has been performed since about 1980 and became fully three dimensional in respect to all important processes around 1998 when sophisticated 3D-simulators with migration were published.