

Compaction of sedimentary rocks

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Abstract

Burial compaction of sedimentary lithotypes results in changes to rock densities. For any pure lithotype, these changes are described and modelled by a porosity function:

$$\rho_b(z) = \rho_{Fr} + (\rho_{fl} - \rho_{Fr})\phi(z)$$

Porosity varies in response to changes in maximum effective stress, generally as an exponential decay function. This porosity function may be modified to incorporate thermo-kinetic and chemical processes. In recent years, various workers have developed and published porosity functions describing compaction in several major lithotypes.

Most rock sequences consist of mixtures of lithotypes. The volumetric proportions of principal lithotypes can be estimated from wireline log data. In mixed lithology sequences, the volumetric and density consequences of burial compaction are estimated by weighted summation of changes to each lithotype present:

$$\rho_b(z) = \sum_{i=1}^{n+m} [v_i \rho_i(z) + \phi_i(z) \rho_{fl}]$$

Systematic variations in rock density computed in this manner are used as a key to detailed analysis and prediction of other sequence attributes which may be of great technical and commercial interest. These include acoustic performance prediction, hydrocarbon generation prediction and primary migration modelling, and sedimentary basin and hydrocarbon system geometric modelling.

Introduction

Upon deposition, most sedimentary rocks may be considered as a mixture of clays, non-clay material and fluids. Typical components are:

- clays (both as dispersed and layered clays);
- effectively incompressible grains (sand, silt and shale size);
- deformable (compressible) detrital grains (e.g. glauconite, mud pellets);
- organic debris (both plant and animal matter); and
- calcareous material (including chemical sediments and both macro and micro fossils).

If we estimate the percentages of these components, and we have some knowledge of the compaction behaviour of each component, we can model the volumetric and density changes of the rock that occur as compaction proceeds. Compaction performance may also vary depending on the mode of distribution of components; e.g. dispersed clays within pore spaces in frame-supported quartz sandstones may behave differently to layered clays.

Shale compaction

Numerous workers have observed progressive changes in shale density (and hence porosity) and shale p-wave velocity

with increasing depth of burial. Several quite different mathematical models have been proposed to describe these changes. An exponential decay model, first proposed by Athy (1930), and subsequently proven by Korvin (1984) for a normally compacted "pure" shale sequence (an idealised shale) has been widely accepted.

$$\rho(z) = \rho_{\infty} + (\rho_0 - \rho_{\infty})e^{-kz}$$

where ρ_{∞} is the shale density at infinite (great) depth,

ρ_0 is the density of the pore fluids,

k is a constant, and

z is depth.

Variations in shale compaction performance have led some workers to question the validity of this model, and to seek alternatives.

Most shales are actually complex mixtures of fine-grained materials. Departures from the exponential decay "pure" shale model can be explained by variations in the mixture of clay types in the shale, in the presence and proportions of non layered-clay components, and in the variable response of these components to increasing overburden load and burial depth.

The application of the Korvin compaction response is restricted to layered-clay components. Variations in Korvin's compaction constant k arise due to variations in clay

components and possibly to rates of sedimentation (and hence rates of compactive dewatering). The behaviour of other components is modelled and quantified using other compaction functions. The mixture of fine-grained lithologic components is termed “mudrock”, and the term “shale” refers to Korvin’s “pure” shale - i.e. a wholly layered-clay mudrock.

Multi-component mudrock

If a mudrock is composed of n differing mineralogic components, and we have, for the i th component, total component volume V_i having density ρ_i and made up of solid volume v_i and pore volume ϕ_i , then in volumetric terms:

$$\sum_{i=1}^n V_i = 1$$

$$\sum_{i=1}^n (v_i + \phi_i) = 1$$

and $\sum_{i=1}^n v_i + \phi = 1$

where ϕ is total rock porosity.

Mudrock non-fluid components may be classified as:

- layered clays (principally kaolinite and smectite clays);
- matrix material (finegrained, principally silica and calcareous material); and
- organic debris.

Assuming the porosity is fully fluid-saturated, in volumetric terms we write:

$$v_{cl} + v_{ma} + v_{org} + v_{fluids} = 1$$

where the subscript cl refers to clay component

ma refers to matrix

org refers to organic component

Recognizing that each solid component has an associated porosity within which the fluid components are distributed, this can be written:

$$v_{cl} + \phi_{cl} + v_{ma} + \phi_{ma} + v_{org} + \phi_{org} = 1$$

Mudrocks may also contain pellets and clasts of other fine-grained material. Mud pellets contain a mix of clays, incompressible and organic debris similar to the main volume of mudrock; their volume is distributed proportionately among the other components and their presence is thereafter ignored in the modelling process. In the absence of data allowing a better model, all kerogenous organic debris is treated as a single compaction type, and calcareous macrofossil material is considered as effectively incompressible. Porosity and density of the mix change with depth, and possibly with other factors (e.g. tectonic stress, clay diagenetic dewatering, and presence and volumes of hydrocarbons which are dependent on other factors, such as time and temperature).

In what follows, the response of each component to burial is modelled and the effects are summed to compute a whole-rock response to compaction.

Generalized rock compaction

In response to burial, changes within a unit volume of a pure sedimentary lithotype can be expressed as:

Initial volume: $V_{Lith} = 1$

Separating porosity: $V_{Frame} + \phi = 1$

Where porosity is filled with fluids: $V_{Frame} + V_{Fluids} = 1$

In terms of bulk density: $\rho_{Fr} V_{Fr} + \rho_{fl} V_{fl} = \rho_b$

hence $\rho_{Fr} V_{Fr} + \rho_{fl} (1 - V_{Fr}) = \rho_b$

so $\rho_b = \rho_{Fr} + (\rho_{fl} - \rho_{Fr}) \phi$

(see Figures 1 and 2).

Thus rock component density is a function of porosity, which is observed to vary with depth.

i.e. $\rho_b(z) = \rho_{Fr} + (\rho_{fl} - \rho_{Fr}) \phi(z)$

where z is depth,

ρ_b is bulk density,

subscript Fr refers to the rock frame, and

fl refers to pore fluids.

The precise form of the depth-related porosity function can be expected to vary in response to mineralogy, temperature and pressure. Some porosity variation may also result from chemical changes (reactions resulting in volumetric change, movement of material by solution into and precipitation from circulating pore fluids).

Layered-clay compaction

In the process of establishing a proof of an exponential decay model for shale compaction, Korvin considers a “pure” shale,

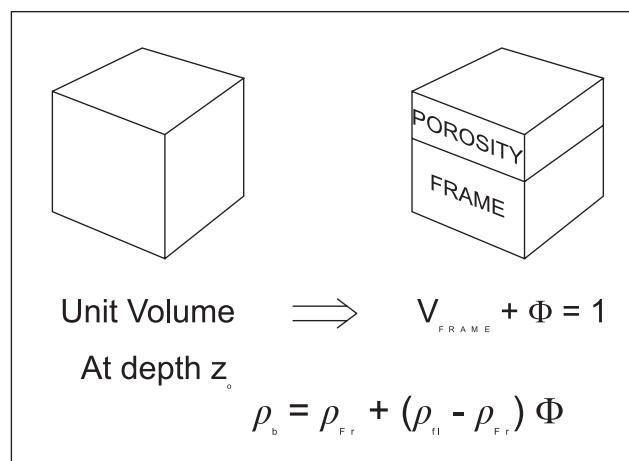


Figure 1: Schematic showing the breakdown of a unit volume of rock into the frame and porosity components.

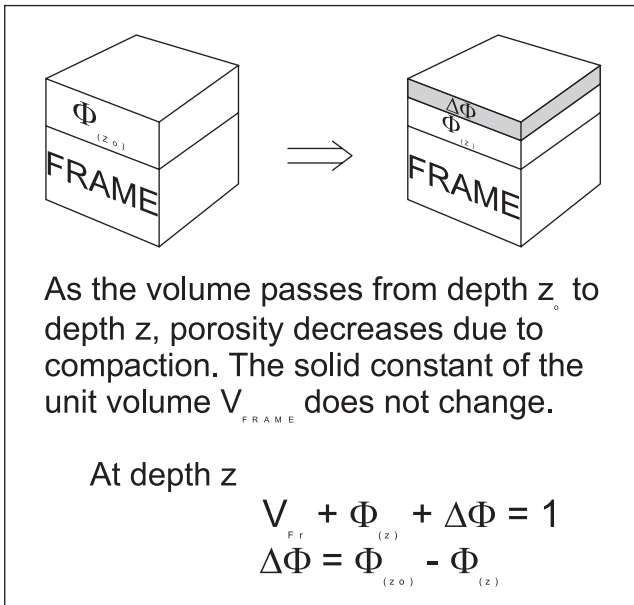


Figure 2: Schematic showing the porosity volume reduction so the rock is progressively buried from depth z_0 to depth z .

without definition, but implies that 1. the non-clay component is absent, 2. there is a single clay type, and 3. all porosity is fluid-filled.

Therefore, for a unit volume: $V_{shale} = 1$
 i.e. $V_{clay} + V_{fluids} = 1$
 and $\phi = V_{fluids}$

As in the above, shale density is a function of porosity, which is observed to vary with depth.

i.e. $\rho_{shale}(z) = \rho_{cl} + (\rho_{fl} - \rho_{cl})\phi(z)$

Korvin (1984) derived a proof that in a normally pressured sequence, shale density increases exponentially with increasing depth of burial, by systematic removal of pore fluids:

$$\rho(z) = \rho_{\infty} + (\rho_0 - \rho_{\infty})e^{-kz}$$

We can equate densities at limits with component densities, and so conclude that Korvin's proof implies that shale porosity declines exponentially with increasing depth of burial:

$$\phi(z) = e^{-kz}$$

This exponential decrease in porosity with depth was first observed and proposed empirically by Athy (1930).

Shale with matrix components

If a matrix (non-clay and non-compressible) component is present in the clay, in volumetric terms:

$$V_{matrix} + V_{shale} = 1$$

$$V_{matrix} + V_{clays} + V_{fluids} = 1$$

In porosity terms, $\phi = 1 - (V_{clays} + V_{matrix})$

and in density terms: $\rho_{cl}V_{cl} + \rho_{fl}V_{fl} + \rho_{ma}V_{ma} = \rho_{shale}$

If the matrix components do not experience significant variation in density during compaction, then for mudrocks containing such materials, the volumetric proportions of the mixture will change with compaction.

For a unit volume passing from burial depth z_0 to depth z , porosity reduces from $\phi(z_0) = e^{-kz_0}$ to $\phi(z) = e^{-kz}$.

The initial volume: $V_{matrix} + V_{clay} + V_{fluids} = 1$

becomes: $V_{matrix} + V_{clay} + \phi(z)$

The difference (volumetric reduction) per unit volume of clay is: $\Delta\phi = \phi(z_0) - \phi(z) = e^{-kz_0} - e^{-kz}$

The new volumes of components are:

$$V_{ma}(z) = V_{ma}(z_0) \cdot \left[1 + \frac{\Delta\phi}{1-\Delta\phi} \right]$$

$$= V_{ma}(z_0) \cdot \left[\frac{1}{1-\Delta\phi} \right]$$

$$V_{cl}(z) = V_{cl}(z_0) \cdot \left[\frac{1}{1-\Delta\phi} \right]$$

$$\phi(z) = e^{-kz}$$

(see Figure 3).

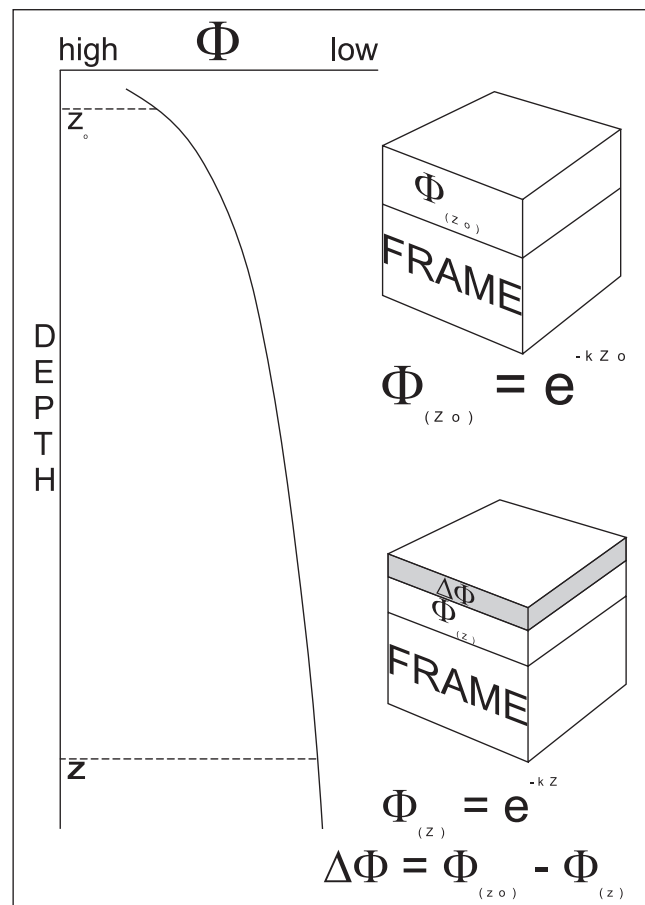


Figure 3: Reduction of porosity follows an exponential trend as a unit volume of rock is progressively buried from depth z_0 to depth z .

The density of the mix at depth z is then:

$$\rho_{shale}(z) = \rho_{cl} V_{cl}(z) + \rho_{fl} e^{-kz} + \rho_{ma} V_{ma}(z)$$

Shale with multiple clay and matrix components

This model can be extended to shale containing a mix of n clay and m matrix types, each having differing densities and compaction responses. Consider a unit volume of mixed clay mudrock composed of n clay types and m matrix types at initial depth z_0 . If the i th component has volume V_i (made up of solid volume v_i and porosity ϕ_i), density ρ_i , and porosity function ϕ_p then:

$$\sum_{i=1}^{n+m} V_i(z_0) = 1$$

For the whole rock

$$\sum_{i=1}^{n+m} [v_i(z_0) + \phi_i(z_0)] = 1$$

$$\rho_b(z_0) = \sum_{i=1}^{n+m} [v_i \rho_i(z_0) + \phi_i(z_0) \rho_{fl}]$$

$$\phi(z_0) = \sum_{i=1}^{n+m} \phi_i(z_0)$$

at depth z $\rho_i(z) = \rho_{i\infty} + (\rho_i - \rho_{i\infty}) \phi_i(z)$
and

$$\rho_b(z) = \sum_{i=1}^{n+m} [v_i \rho_i(z) + \phi_i(z) \rho_{fl}]$$

$$\phi(z) = \sum_{i=1}^{n+m} \phi_i(z)$$

The new component volume is $V_i(z) = v_i + \phi_i(z)$

The component volume reduction is $\phi_i(z_0) = \phi_i(z)$

The initial unit volume is reduced to

$$\sum_{i=1}^{n+m} V_i(z)$$

with total volumetric reduction

$$\Delta\phi = \sum_{i=1}^{n+m} [\phi_i(z_0) - \phi_i(z)]$$

The volume of each component in the unit volume at the new depth is then:

$$V_i(z) = V_i(z_0) \cdot \frac{1}{[1 - \Delta\phi]}$$

with related expressions for the whole rock density and porosity (see Figures 4 and 5).

The above is a generalized model which can be applied to all lithologies. Provided an appropriate porosity function can be defined for each component, volumetric and density changes to the whole rock as a result of compaction can be precisely modelled.

The process can also be inverted. Using this approach, assuming compaction occurs by gravitational compression, rock unit densities and thicknesses at prior depths can be precisely reconstructed.

Compaction porosity functions

Clays

The model of Athy (1930) as applied by Korvin (1984) is applied to compaction of normally pressured layered clays. For each layered clay component, provided Korvin's compaction constant k can be established, clay porosity variations can be modelled:

$$\phi_i(z) = e^{-kz}$$

Quartz sandstones

Since the initial work of Athy (1930), porosity reduction in quartz sandstones resulting from increasing depth of burial has been widely studied. Core data from the US Gulf Coast sandstone reservoirs attributed to Dickinson (1983) (Figure 3b. in Law et al 1983) show close agreement with a simple exponential function:

$$\phi(z) = 2.5 + 37.5e^{-0.5z}$$

from surface to depths in excess of 8 km (see Table 1).

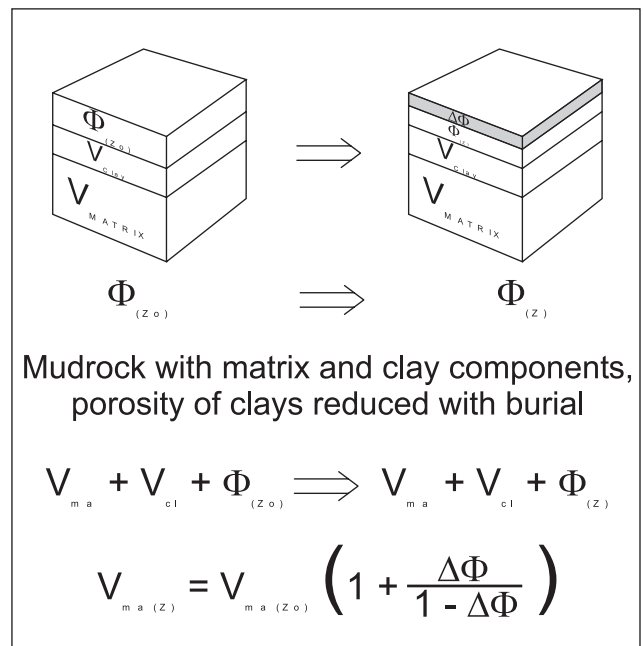


Figure 4: Schematic showing the breakdown of a unit volume of rock into its frame components.

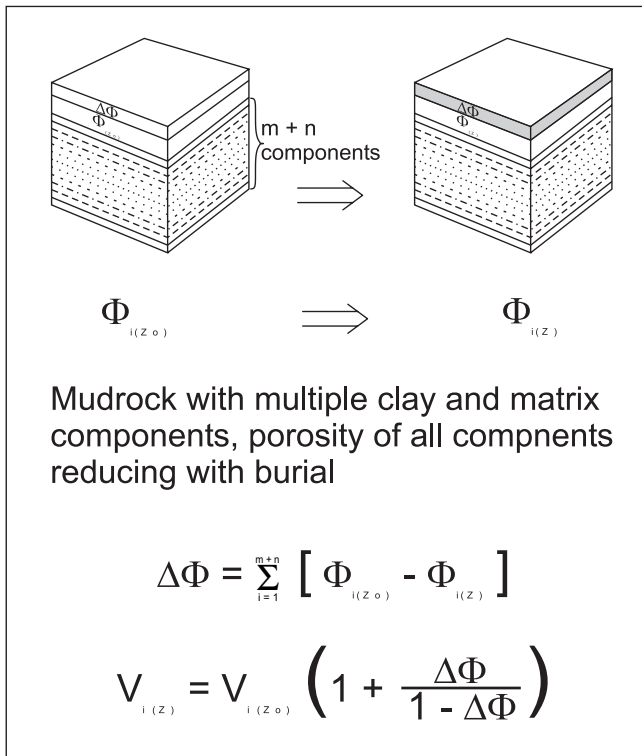


Figure 5: Schematic of multi-component lithotype having n clay types and m matrix types.

In a more detailed model, Lander and Walderhaug (1999) consider reduction in quartz sandstone intergranular volume (IGV) as the sum of compaction effects in response to increasing effective stress, plus cementation effects in response to changes in the chemical and physical environment. Reduction in IGV (the sum of porosity, matrix and cement volumes) due to compaction generally follows an exponential decline. Their function is:

$$IGV = IGV_f + \phi_0 + m_0 - IGV_f e^{-\beta\sigma_{es}}$$

where IGV_f is the intergranular volume at a stable packing configuration,

ϕ_0 is the depositional porosity,

m_0 is the initial matrix volume,

β is the exponential rate of IGV decline, and

σ_{es} is the maximum effective stress

The rate of IGV reduction can be slowed by early-formed chemical quartz cementation prematurely increasing the rock frame strength. The chemical aspects of cementation are principally dependent on the time-temperature history of the rocks, and are considered separately.

Vernik (1998) recognizes two stages of porosity reduction in sandstones. Immediate post-depositional porosity decreases rapidly from approximately 40% to approximately 30% due to packing rearrangement. Subsequent porosity reduction occurs more slowly. Vernik's work relates sandstone porosity to sonic velocity, but not to maximum burial depth.

Carbonates

Porosity reduction in carbonate sediments is complex. A wide porosity range with depth is possible, depending on the type of initial deposit (ooze/chalk versus coarser crystalline material) (Grutzner and Mienert, 1999) and the post-depositional diagenetic and thermal history (Hamilton, 1976), including presence and timing of charge of hydrocarbons (Brasher and Vagle, 1996).

The mode of initial carbonate deposition has changed significantly through geologic time. Prior to the evolutionary development of significant numbers of species with calcareous exoskeletons (Ordovician to Devonian), carbonate sedimentation occurred by chemical precipitation. Due to their age and initial mode of deposition, porosity development and porosity trends within these sediments are now dominated by solution and dolomitization. For modelling purposes, we regard these sediments as normally pressured carbonates (Category I carbonates of Brasher and Vagle, 1996).

Since Devonian time, carbonate sediments have also included a range of commonly coarse-grained skeletal debris, often intimately mixed with fine-grained quartzose clastic debris and chemical carbonates. These coarse-grained carbonate and mixed carbonate rocks are also treated as Category I rocks.

Since early Cretaceous time there has been a significant increase in the diversity and volume of pelagic marine microorganisms with calcareous skeletons. Since that time, marine carbonate sedimentation has been dominated by the development of marine calcareous oozes which, during burial, evolve into chalks and ultimately limestones. Very large volumes of such sediments have formed, and continue to form, in most marine basins. When deeply buried, these

Depth (km)	Porosity Cat I	Computed Porosity
0.00	72	72.0
0.10	63	66.0
0.25	56	57.9
0.50	47	46.6
1.00	34	30.5
1.50	24	20.1
2.00	14	13.6
2.50	8	9.4
3.00	3	6.7
3.50	2	5.0
4.00	2	3.9
7.00	2	2.1

Table 1: Sandstone porosity reduction with increasing burial.

Depth (km)	Observed Porosity	Computed Porosity
0	40.0	40.0
1	24.0	25.2
2	16.0	16.3
3	11.0	10.9
4	8.0	7.6
5	6.0	5.6
6	4.5	4.4
7	3.5	3.6
8	2.8	3.2
9		2.9
10		2.8

Table 2: Computation of porosity of Category 1 carbonates.

sediments commonly contain hydrocarbons, either due to conversion of contained carbon compounds, or due to invasion by migrating hydrocarbons.

Depending on their burial, post-burial and hydrocarbon charge histories, these sediments can exhibit a wide range of porosity trends. In the deeper basins, these sediments may be principally mass flow deposits in which the basin is predominantly filled with debris initially deposited in shallower water on the basin shelves (Brasher and Vagle, 1996). These mass flow deposits are termed Category III rocks (Brasher and Vagle, 1996). They commonly show significantly enhanced primary porosity, which may be preserved by early emplacement of hydrocarbons, and by restricted circulation of pore fluids (evidenced by development of overpressured compartments).

Such overpressured, high porosity, hydrocarbon-bearing chalk reservoirs can be of great commercial significance, but are unusual in the broader geologic context. We model porosity evolution in normally pressured carbonate sequences (Category I) using an exponential compaction function based on the data of Hamilton (1973) and Grutzner and Mienert (1999):

$$\phi(z) = 2 + 70e^{-0.9z}$$

This yields carbonate porosities close to those expected in the near-surface and at depth, but tends to slightly overestimate midrange porosities (see Table 2).

Organic debris

Burial to significant depths is usually associated with both progressively increasing temperature and long periods of time. These time-temperature effects cause progressive alteration to the kerogen present, and lead to the generation of hydrocarbon liquids and gas. A large volume of data on organic maturation and hydrocarbon generation processes exists, but little data is available on changes to density and

volume of the various types of organic debris during that process. Knowledge of the thermal history of the sequence, its relationship to the burial history, and their combined effects on the alteration of organic material, may be required if changes to the volume and density of organic components are to be modelled.

The data of Law et al. (1983) is used as a guide to the changes in coal rank and vitrinite reflectance that might take place during compaction of organic material. In the absence of other data, all organic debris is treated as a single type, and coal-based volumetric relationships are applied to all organics. The relationships developed herein should be considered as approximations only; this is an area where further laboratory and field studies would be of great benefit.

Compactive dewatering of coal results in systematic reduction of moisture content, somewhat less rapid reduction in volatile matter content, and increased fixed carbon content. The rate of these changes is dependent on the chemical make-up of the original organic debris, on the thermal history, and on the duration of exposure to elevated temperatures. These variables are not taken into account in the work of Law et al. (1983).

This scheme does not relate rank to coal density or compaction volume. Consideration of the density of clean coal components (carbon, volatile matter, moisture) also indicates that coal density may change only slightly with compaction, even though the coal may undergo significant volume change.

Coal is regarded as a mixture of fixed carbon, volatile matter, mineral matter (ash) and water. For a clean (ash free) coal undergoing compactive dewatering:

$$\rho(\text{coal}) = \rho(\text{fc}) \cdot V(\text{fc}) = \rho(\text{vm}) \cdot V(\text{vm}) + \rho(\text{fl}) \cdot V(\text{fl})$$

(Law et al. 1983, fig 2).

Assuming that changes in coal density with increasing metamorphism are due to loss of water and volatiles, using the data of Law et al (1976, fig. 2) changes in density of volatile matter can be estimated:

1. at low rank (lignite), coal density is approximately 1.1 (Gearhart, 1986), and:

$$\rho(\text{coal}) = \rho(\text{fc}) \cdot V(\text{fc}) + \rho(\text{vm}) \cdot V(\text{vm}) + \rho(\text{fl}) \cdot V(\text{fl})$$

[assuming fixed carbon density = 1.55, which is close to that of anthracite (1.6), and the contained water is low salinity (assume 10000 ppm chloride). (The data of Law et al. suggests this is a reasonable estimate of salinity for water included in the coal.)]

which becomes:

$$1.1 = 1.55 * 0.27 + 0.23 * \rho(\text{vm}) + 1.01 * 0.$$

$$\text{hence } \rho(\text{vm}) = 0.786$$

2. at higher rank (low volatile bituminous), coal density is approximately 1.35, so:

$$1.35 = 1.55 * 0.77 + 0.17 * \rho(vm) + 1.01 * 0.07$$

$$\text{hence } \rho(vm) = 1.227$$

This assumes average values, which may be subject to considerable error, particularly in regard to coal densities. On the available data, it seems the density of coal volatile matter only increases slightly during metamorphism, even though the volume may reduce significantly.

Over the main range of coal compaction volumetric changes, coal fixed carbon density is assumed to remain nearly constant, and total density changes are the result of changing volumes of contained water, with modest changes to the density of the volatile matter component. A density of 1.55 is used for fixed carbon, and an exponential decay function for density of volatile matter.

$$\rho_{vm} = 0.786 + (1.227 - 0.786)e^{-\left[\frac{2.8-R_0}{R_0}\right]}$$

where R_0 is vitrinite reflectance.

Figures 2 and 3 of Law et al. (1983) can be used to develop simple empirical volumetric relationships between maximum burial depth, coal fixed carbon, moisture and vitrinite reflectance in the Green River Basin, Wyoming. In approximate terms:

$$FC = 32 + 65 * (1 - e^{-0.25z})$$

$$\text{Moisture} = 35 - 32 * (1 - e^{-0.7z})$$

$$R_0 = 0.3 + 0.16z + 0.01z^2 + .002z^3$$

Where FC = Fixed Carbon (percentage),

Z = maximum burial depth, and

Moisture is in percent

The computed vitrinite reflectance is applied to derive density of the volatile matter component, and then to continuously compute coal density:

$$\rho(\text{coal}) = 1.55 * V(fc) + \rho_{vm} * V(vm) + 1.01 * V(fl)$$

These relationships assume a known thermal gradient remaining constant over time. With suitable thermal history data, it should be possible to model the thermal and burial history of specific sedimentary units, and modify the above relationships to better reflect the combined burial, thermal and time effects.

It follows that the physical properties of coal components only change slowly during compaction. Volumetric changes principally result from loss of moisture; if the coal frame and contained moisture/volatiles are of similar physical properties, moisture/volatiles expulsion will result from load-induced collapse of the frame, with little change to the density of the whole rock.

The volumetric change can be calculated from changes to the volume of moisture and volatiles present. These volumes may be calculated from the above. As the coal passes from depth z_0 to depth z , volume of fixed carbon increases:

$$V_{FC}(z) - V_{FC}(z_0) = 0.65 * (e^{-0.25z} - e^{-0.25z_0})$$

This is the amount by which the combined volumes of moisture and volatile matter decrease i.e. the volumetric reduction per unit volume.

The ratio of the new volume to the old is:

Rank ASTM	Max. Burial (km)	Fixed Carbon %	Moisture %	Volatile Matter %	R_0 %	Rank (S)
Lignite	0.00	32.0	35.0	33.0	0.3	3.5
Sub-Bitum C	0.60	41.1	24.0	34.9	0.4	7.4
Sub-Bitum A	1.22	49.1	16.6	34.3	0.5	10.1
HV Bitum C	1.90	56.6	11.5	32.0	0.7	12.1
HV Bitum A	2.45	61.8	8.8	29.5	0.8	13.3
HV Bitum A	3.35	68.9	6.1	25.1	1.1	14.8
MV Bitum	3.80	71.9	5.2	22.9	1.2	15.4
LV Bitum	4.60	76.4	4.3	19.3	1.6	16.3
Semi-Anthracite	5.50	80.6	3.7	15.8	2.1	16.9
Anthracite	6.25	83.4	3.4	13.2	2.6	17.4

Table 3: Changes in coal components and properties with increasing burial depth.

$$\frac{VFC(z)}{VFC(z_0)} = \frac{[0.32 - 0.65 \cdot (1 - e^{-0.25z})]}{[0.32 - 0.65 \cdot (1 - e^{-0.25z_0})]}$$

As coal passes from lignite to low volatile bituminous, fixed carbon percentage increases from approximately 30% to 75%, and the volume loss is approximately 60%. This implies that a lignite 12 m in thickness near surface will transform into a bituminous coal approximately 4.8 m in thickness at burial depth of approximately 4.5 km.

Coal porosity may increase in the advanced stages of metamorphism (Garcia-Gonzalez et al., 1996), due to the development of secondary porosity. This development is apparently related to generation of gas, and its migration from the coal. This development should be restricted to coal lithologies, and should not occur in organic matter dispersed in sediments.

In the absence of other data, the compaction performance of coal is applied to all organic components, at all scales. The volume of total organic carbon present in a sediment is equated to the volume of coal fixed carbon; this is then used to estimate the organic content at lesser compaction levels.

Overburden load and rock stress

In the above model, mechanical compaction is presumed to result from the increasing overburden load as sediments are progressively buried. Gravitational loading produces a predictable rock frame stress, which may be modified by local tectonic stresses to produce a more complex total mechanical stress. Below the water table, porous rocks are fluid saturated, and pressures in the pore fluids increase progressively with increasing depth below the water table. The pressure gradient is normally that of a water column; the density of the fluid column varies with salinity, but within the normal range of variation, the rocks are said to be normally pressured.

The effective stress in a rock is (Khavari Khorasani and Michelsen, 1994):

$$\sigma_{es} = \sigma - \phi_f - \rho_f g z$$

where σ is the total pressure,

ϕ_f is the deviation from hydrostatic pressure,

ρ_f is the fluid density,

g is acceleration of gravity, and

z is the height of the sediment column

Hence in all of the above discussion on mechanical aspects of compaction, depth of burial should, more correctly, be replaced by an effective stress term.

Various conditions can lead to increases in the pore fluid pressure; such rocks are said to be overpressured or abnormally pressured. Increased pore pressure yields reduced effective stress. Various rock properties, including compaction and elastic wave propagation behaviour, respond to changes in effective stress.

Thermo-kinetically influenced chemical changes

Progressively increasing depth of burial is generally associated with increasing temperature. The combined temperature of a depositional unit, and the duration in time of exposure to that temperature, control many aspects of chemical alteration of the compacting rock. These include chemical solution and recrystallization of calcite, clays and silica infilling pore spaces in reservoir lithologies, thermally driven dewatering of hydrous clays, and generation of gas and liquid hydrocarbons from organic matter.

Hydrocarbons generation

The thermal profile can be measured or estimated. If the temperature history of each depositional unit can be established in suitable time increments (e.g. thermal history since beginning of Triassic time could be modelled in 25 equal increments each of 10 million years duration, or alternatively, the time divisions can be made to coincide with major depositional increments), then a maturation parameter C can be computed for each unit (De Bremaecker, 1983):

$$C = \ln \int_0^t 2^{0.17T} dt$$

where t is time in millions of years

T is temperature in degrees Celsius

Estimation of maximum effective vitrinite reflectance R_o then follows.

$$R_o \approx e^{(0.173C - 2.242)}$$

When R_o is computed in this manner, the principal phase of oil generation begins at approximately $R_o = 0.6$, and the last phase of dry gas generation has ended by $R_o = 3.4$ approximately (De Bremaecker, 1983). Under normal rates of burial, and normal ranges of thermal gradients, the principal phase of hydrocarbon generation begins at between about 75°C and 130°C (Hunt, 1979).

The process of hydrocarbons generation is thermally controlled. If the sediment is sufficiently rich in total organic carbon (TOC ≥ 0.6 approximately) then, once begun, hydrocarbon generation proceeds relatively independently of pressure. Depending on the type of kerogen present and TOC richness, substantial volumes of hydrocarbons may be generated.

Clay dewatering

In many sequences, depositional clays contain significant amounts of hydrous clays (smectites). These clays may release substantial volumes of water of hydration when heated during the burial/compaction process (Bruce, 1984; Clauer et al., 1999). The release of water of hydration is thermally

triggered, and occurs at effectively the same time and temperature as, or a little later than, the onset of the principal phase of hydrocarbon generation. The clay dewatering reaction consumes K-feldspar and mica, and liberates illite, chlorite and silica as well as the water of hydration (Bruce, 1984).

The water liberated in this process is initially released from the clay crystal structure, and injected into the shale inter-particle porosity. It mingles with the residual connate water. Provided the bulk of this water is, in the short term, retained within the shale, the shale pore pressure rises, reducing the effective stress of the rock and reducing the density of the rock (Bruce, 1984).

Silica cementation

Walderhaug (1996) and Lander and Walderhaug (1999) presented a model for porosity reduction in quartz sandstones resulting from thermally driven silica cementation as a modifier of porosity reduction due to compaction. Volumetric consequences of porosity reduction arising from silica cementation are complex (Lander and Walderhaug, 1999). Early silica cementation can substantially increase the stiffness of the rock, and reduce the subsequent effects of compaction. Other difficulties may arise from chemical change. For example, if significant volumes of chlorite and silica are liberated from shales during the process of clay dewatering (Bruce, 1984) and are then carried into the sandstone during the process of primary migration (see below), significant silica cementation can result, with porosity reduction unrelated to volumetric change.

In the present model, quartz sandstone porosity reduction is regarded as a process of volumetric re-arrangement within a closed system. An exponential model is used to describe the porosity and hence volumetric trends of Dickinson (1983) in Law et al. (1983).

Consequences and applications of the compaction model

Process and timing of primary migration of hydrocarbons

During the mechanical compaction of rock components, pore volumes are reduced. Burial compaction is usually associated with the thermally driven process of hydrocarbon generation, once the required thermal conditions are met. Both process may be accompanied by smectite diagenesis leading to liberation of significant volumes of water which mingle with the pore fluids and compete for available pore volume. These conditions can lead to abrupt and substantial increases in pore pressure, with apparent reversal of compaction trends.

In petroleum source rocks, hydrocarbons originate from thermal alteration of the organic components. Prior to primary migration, these occupy some of the clay and non-clay pore volume by solution in the pore water. Once begun, generation

may proceed, with hydrocarbons progressively saturating the pore fluids, with little effect on pore pressure until the pore fluid system is fully saturated. Further generation results in development of a separate hydrocarbon phase, with a resultant increase in pore pressure. Pore liquids (connate water, clay released water of hydration, and hydrocarbon liquids) accept increasing volumes of lighter hydrocarbons into solution as the pore pressure rises.

Given appropriate thermal conditions, hydrocarbon generation and clay dewatering will proceed independently of confining pressures, until the accumulating pore pressure exceeds the retention capacity of the shale. At this point the seal fails, and fluids are expelled. This failure may be accelerated by ongoing clay dewatering, and by changes to the wettability of the rock in response to the changing pore fluid mixture. The failure may start along an anisotropy in the rock (bedding or structural), but will not propagate unless there is a fluid flow path which will allow pressure release.

Failure, allowing release of pressure from the pore system, results in rapid local increase in pore fluid pressure gradients in the vicinity of the initial failure. This increase in pressure gradients causes pervasive microfracturing of the pressurized rock, with rapid expulsion of fluids. Once initiated, the fluid flow is driven by the energy contained in the pressurized pore fluids containing dissolved gases. Microfractures propagate until an effective drainage system develops throughout the entire rock.

Reduction in pore pressure leads to exsolution of hydrocarbons from the pore water; expansion of liberated gases tends to maintain pressures, and drive a pulse of migrating hydrocarbons from the source rock. Once begun, the process will continue until the pore pressure falls sufficiently that the sealing capacity of the source rock is at least partly restored by closure of the microfracture system.

Once fluid flow through the microfracture system stops, much of the sealing capacity of the rock restores over time, by cementation. The process of generation and accumulation within the source rock proceeds and the process is repeated. Primary migration from such source rocks is thus pulse-like.

The mix of accumulating hydrocarbons and pore water will change over time, as the availability and volume of clay water and mix of hydrocarbons being generated changes during the process of thermal maturation. Initial migration products will be light oils and gases, accompanied by potentially large volumes of water. Separation of phases will subsequently occur in reservoirs, under more normal pressure regimes. Depending on the source kerogen type, subsequent pulses will progressively carry more hydrocarbon liquids; in the late stages, remnant oil and bitumen may be left on microfracture surfaces. Source rocks rich in oil-prone kerogen, but low in smectite content (either due to non-deposition or thermal depletion of the initial bound water) may act as low grade reservoirs (self-sourcing reservoirs) by development of an oil-saturated microfracture system.

Early formed liquid hydrocarbons may, if later subjected to thermal cracking, degrade to bitumen and lighter hydrocarbons. This may occur in either source rocks or reservoirs. Under the correct thermal conditions, this process can lead to microfracturing even in reservoir lithologies (Marquez and Mountjoy, 1996).

Using the above approach, compaction and thermal history can be modelled. The timing of generation within, and primary migration of hydrocarbons from source rocks can be predicted. Source/seal/reservoir geometries of hydrocarbons systems can be reconstructed as they were at the time of maximum primary migration. This yields an improved basis for the search for subtle, semi-stratigraphic accumulations of oil and gas.

The presence of significant overpressures in potential source rock sequences indicates that the sequence is in the process of generative accumulation, wherein the hydrocarbons are stored in the source rock pore fluids. The presence of such overpressures is a strong indication that the sequence permeability is sufficiently low that long-term fluid flow through the sequence is not taking place. Reservoir lithologies within such overpressured sequences are unlikely to sustain commercial production, even though initial production might be encouraging.

Seismic performance modelling

Using this compaction model, knowledge of the principal lithologic components in a sequence allows prediction of density changes with depth. Seismic p-wave velocities can be predicted (Wiltshire and Huggard, APPEA 2000 Conference Journal, in press).

Using only compaction trends and generalized estimates of lithology yields relatively low frequency estimates of velocity. Rock porosity derived from wireline log data can provide the desired higher frequency component. When the low frequency component is modified by a transform of the log-based porosity, the resultant composite velocity function is virtually indistinguishable from an acquired sonic log. A synthetic sonic log of this type and quality provides a potentially valuable tool in seismic studies, in linking well sections to seismic data. This allows better use of data from older wells, or wells in which no sonic log was run. Even very old well data may be used.

This sonic log modelling technique has potentially great impact in drilling planning and management. Using only MWD resistivity data, sonic and seismic interpretation modelling can be carried out during drilling. Significant savings in operational procedures and improvements in drilling and engineering safety can follow.

Operational considerations and requirements

Depending on provenance and depositional environment, significant variation in clay types is possible. Bruce (1984)

reports substantial differences between clays in average Gulf Coast and Niger delta shales. Using a combination of spectral gamma ray and litho-density log data, it may be possible to identify dominant clay types present in shales, and to associate these log responses with clay types identified by X-ray and chemical analyses. Wireline log data might then be used to identify and quantify clay types.

Characterization of Korvin's compaction constant k for each clay type is desirable. In the absence of such data, the data of Bruce (1984) and Clauer et al (1999) suggest that within a specific geologic setting (basin and depositional unit) the ratio of clay types present should vary only slightly. Mixed-clay compaction behaviour may be adequately characterized by a hybrid compaction constant applied to the total volume of clay present. Thermally induced changes in clay type may also lead to changes in compaction performance.

Continuous quantitative interpretation of lithotypes from wireline log data, using neural net techniques, has been demonstrated (Westphal and Bornholdt, 1996; Westphal and Aigner, 1997). Once compaction behaviour has been characterized for the lithologies present, such a method should allow detailed and precise reconstruction of volumetric changes which have occurred in the sequence during compaction.

Better definition of volumetric behaviour of organic materials, including coals, during compaction would also improve the quality of volumetric modelling.

Conclusions

Modelling of volumetric changes which occur during compaction is possible for most common sedimentary rock types. Volumetric addition allows us to generalize this model, allowing application to mixed lithologies. The process can be inverted, and applied to decompaction computations. This yields potentially significant improvements in reconstruction of the geometric history of sedimentary sequences.

When linked to hydrocarbon maturation models, it is possible to explain and model the process of primary migration of hydrocarbons from source rocks. The process of primary migration is not a steady-state process. The combined processes of hydrocarbon generation and sequence dewatering (including thermal dewatering of bound water from layered clays) lead to accumulation of stored energy in the pore fluid system, followed by relatively rapid expulsion of fluids from the source rocks as a pulse. Once this stored energy is released, permeability falls and the process repeats.

This understanding of the compaction process leads to an improved sonic performance model. The technique allows better use of wells with no or poor quality sonic log data in the modern exploration environment, and improved economics and safety in drilling planning and management.

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